Bioinformatics Toolbox 2

Reference

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Bioinformatics Toolbox Reference

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Functions — By Category

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`cleave`	Cleave amino acid sequence with enzyme
`evalrasmolscript`	Send RasMol script commands to Molecule Viewer window
`isoelectric`	Estimate isoelectric point for amino acid sequence
`molviewer`	Display and manipulate 3-D molecule structure
`molweight`	Calculate molecular weight of amino acid sequence
`pdbdistplot`	Visualize intermolecular distances in Protein Data Bank (PDB) file
`proteinplot`	Characteristics for amino acid sequences
`proteinpropplot`	Plot properties of amino acid sequence

`ramachandran`	Draw Ramachandran plot for Protein Data Bank (PDB) data
`rebasecuts`	Find restriction enzymes that cut protein sequence

Profile Hidden Markov Models

`gethmmalignment`	Retrieve multiple sequence alignment associated with hidden Markov model (HMM) profile from PFAM database
`gethmmprof`	Retrieve hidden Markov model (HMM) profile from PFAM database
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Microarray File Formats

`affyprobeseqread`	Read data file containing probe sequence information for Affymetrix GeneChip array
`affyread`	Read microarray data from Affymetrix GeneChip file (Windows 32)
`agferead`	Read Agilent Feature Extraction Software file
`celintensityread`	Read probe intensities from Affymetrix CEL files (Windows 32)
`galread`	Read microarray data from GenePix array list file
`geosoftread`	Read Gene Expression Omnibus (GEO) SOFT format data
`getgeodata`	Retrieve Gene Expression Omnibus (GEO) Sample (GSM) data
`gprread`	Read microarray data from GenePix Results (GPR) file
`imageneread`	Read microarray data from ImaGene Results file
`sptread`	Read data from SPOT file

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Mass Spectrometry File Formats, Preprocessing, and Visualization

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`msppresample`	Resample mass spectrometry signal while preserving peaks

`msresample`	Resample mass spectrometry signal
`mssgolay`	Smooth mass spectrum with least-squares polynomial
`msviewer`	Explore mass spectrum or set of mass spectra
`mzxml2peaks`	Convert mzXML structure to peak list
`mzxmlread`	Read mzXML file into MATLAB as structure

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Functions — Alphabetical List

aa2int

Purpose

Convert amino acid sequence from letter to integer representation

Syntax

```
SeqInt = aa2int(SeqChar)
```

Arguments

SeqChar	Either of the following: • Character string of single-letter codes specifying an amino acid sequence. See the table Mapping Amino Acid Letters to Integers on page 2-2 for valid codes. Unknown characters are mapped to `0`. Integers are arbitrarily assigned to IUB/IUPAC letters. • Structure containing a `Sequence` field that contains an amino acid sequence, such as returned by `fastaread`, `getembl`, `getgenpept`, or `getpdb`.

Return Values

SeqInt	Row vector of integers specifying an amino acid sequence.

Mapping Amino Acid Letters to Integers

Amino Acid	Code	Integer
Alanine	A	1
Arginine	R	2
Asparagine	N	3
Aspartic acid (Aspartate)	D	4
Cysteine	C	5
Glutamine	Q	6
Glutamic acid (Glutamate)	E	7
Glycine	G	8
Histidine	H	9

Amino Acid	Code	Integer
Isoleucine	I	10
Leucine	L	11
Lysine	K	12
Methionine	M	13
Phenylalanine	F	14
Proline	P	15
Serine	S	16
Threonine	T	17
Tryptophan	W	18
Tyrosine	Y	19
Valine	V	20
Aspartic acid or Asparagine	B	21
Glutamic acid or glutamine	Z	22
Any amino acid	X	23
Translation stop	*	24
Gap of indeterminate length	-	25
Unknown or any character or symbol not in table	?	0

Description

`SeqInt = aa2int(SeqChar)` converts `SeqChar`, a string of single-letter codes specifying an amino acid sequence, to `SeqInt`, a `1`-by-`N` array of integers specifying the same amino acid sequence. See the table Mapping Amino Acid Letters to Integers on page 2-2 for valid codes.

Examples

Converting a Simple Sequence

Convert the sequence of letters `MATLAB` to integers.

```
SeqInt = aa2int('MATLAB')

SeqInt =

    13     1    17    11     1    21
```

Converting a Random Sequence

Convert a random amino acid sequence of letters to integers.

1 Create a random character string to represent an amino acid sequence.

```
SeqChar = randseq(20, 'alphabet', 'amino')

SeqChar =

   dwcztecakfuecvifchds
```

2 Convert the amino acid sequence from letter to integer representation.

```
SeqInt = aa2int(SeqChar)

SeqInt =

  Columns 1 through 13
     4   18    5   22   17    7    5    1   12   14    0    7    5

  Columns 14 through 20
    20   10   14    5    9    4   16
```

See Also

Bioinformatics Toolbox functions: aminolookup, int2aa, int2nt, nt2int

Purpose Convert amino acid sequence to nucleotide sequence

Syntax

```
SeqNT = aa2nt(SeqAA)
aa2nt(..., 'PropertyName', PropertyValue,...)
aa2nt(..., 'GeneticCode', GeneticCodeValue)
aa2nt(..., 'Alphabet' AlphabetValue)
```

Arguments

SeqAA	Amino acid sequence. Enter a character string or a vector of integers from the table. Examples: `'ARN'` or `[1 2 3]`
GeneticCodeValue	Property to select a genetic code. Enter a code number or code name from the Genetic Code on page 2-5 table below. If you use a code name, you can truncate the name to the first two characters of the name.
AlphabetValue	Property to select a nucleotide alphabet. Enter either `'DNA'` or `'RNA'`. The default value is `'DNA'`, which uses the symbols `A`, `C`, `T`, `G`. The value `'RNA'` uses the symbols `A`, `C`, `U`, `G`.

Genetic Code

Code Number	Code Name	Code Number	Code Name
1	Standard	12	Alternative Yeast Nuclear
2	Vertebrate Mitochondrial	13	Ascidian Mitochondrial
3	Yeast Mitochondrial	14	Flatworm Mitochondrial

Code Number	Code Name	Code Number	Code Name
4	Mold, Protozoan, Coelenterate Mitochondrial, and Mycoplasma /Spiroplasma	15	Blepharisma Nuclear
5	Invertebrate Mitochondrial	16	Chlorophycean Mitochondrial
6	Ciliate, Dasycladacean, and Hexamita Nuclear	21	Trematode Mitochondrial
9	Echinoderm Mitochondrial	22	Scenedesmus Obliquus Mitochondrial
10	Euplotid Nuclear	23	Thraustochytrium Mitochondrial
11	Bacterial and Plant Plastid		

Description

`SeqNT = aa2nt(SeqAA)` converts an amino acid sequence (*SeqAA*) to a nucleotide sequence (*SeqNT*) using the standard genetic code. In general, the mapping from an amino acid to a nucleotide codon is not a one-to-one mapping. For amino acids with more than one possible nucleotide codon, this function selects randomly a codon corresponding to that particular amino acid.

For the ambiguous characters `B` and `Z`, one of the amino acids corresponding to the letter is selected randomly, and then a codon sequence is selected randomly. For the ambiguous character `X`, a codon sequence is selected randomly from all possibilities.

`aa2nt(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`aa2nt(..., 'GeneticCode', GeneticCodeValue)` selects a genetic code (*GeneticCodeValue*) to use when converting an amino acid sequence (*SeqAA*) to a nucleotide sequence (*SeqNT*).

`aa2nt(..., 'Alphabet' AlphabetValue)` selects a nucleotide alphabet (*AlphabetValue*).

Standard Genetic Code

Amino Acid		Amino Acid	
Alanine (A)	GCT, GCC, GCA, GCG	Phenylalanine (F)	TTT, TTC
Arginine (R)	CGT, CGC, CGA, CGG, AGA, AGG	Proline (P)	CCT, CCC, CCA, CCG
Asparagine (N)	ATT, AAC	Serine (S)	TCT, TCC, TCA,TCG, AGT, AGC
Aspartic acid (Aspartate, D)	GAT, GAC	Threonine (T)	ACT, ACC, ACA, ACG
Cysteine (C)	TGT, TGC	Tryptophan (W)	TGG
Glutamine (Q)	CAA, CAG	Tyrosine (Y)	TAT, TAC
Glutamic acid (Glutamate, E)	GAA, GAG	Valine (V)	GTT, GTC, GTA, GTG
Glycine (G)	GGT, GGC, GGA, GGG	Aspartic acid or Asparagine	B—random codon from D and N

Amino Acid		Amino Acid	
Histidine (H)	`CAT, CAC`	Glutamic acid or Glutamine	Z—random codon from `E` and `Q`
Isoleucine (I)	`ATT, ATC, ATA`	Unknown or any amino acid	`X random codon`
Leucine (L)	`TTA, TTG, CTT, CTC, CTA, CTG`	Translation stop (*)	`TAA, TAG, TGA`
Lysine (K)	`AAA, AAG`	Gap of indeterminate length (-)	`---`
Methionine (M)	`ATG`	Any character or any symbol not in table (?)	`???`

Examples

1 Convert an amino acid sequence to a nucleotide sequence using the standard genetic code.

```
aa2nt('MATLAB')

Warning: The sequence contains ambiguous characters.
ans =
ATGGCAACCCTGGCGAAT
```

2 Use the Vertebrate Mitochondrial genetic code.

```
aa2nt('MATLAP', 'GeneticCode', 2)

ans =
ATGGCAACTCTAGCGCCT
```

3 Use the genetic code for the Echinoderm Mitochondrial RNA alphabet.

```
aa2nt('MATLAB','GeneticCode','ec','Alphabet','RNA')

Warning: The sequence contains ambiguous characters.
ans =
AUGGCUACAUUGGCUGAU
```

4 Convert a sequence with the ambiguous amino acid character `B`.

```
aa2nt('abcd')

Warning: The sequence contains ambiguous characters.
ans =
GCCACATGCGAC
```

See Also

Bioinformatics Toolbox functions: `geneticcode`, `nt2aa`, `revgeneticcode`, `seqtool`

MATLAB function: `rand`

aacount

Purpose

Count amino acids in sequence

Syntax

```
Amino = aacount(SeqAA)
aacount(..., 'PropertyName', PropertyValue,...)
aacount(..., 'Chart', ChartValue)
aacount(..., 'Others', OthersValue)
aacount(..., 'Structure', StructureValue)
```

Arguments

SeqAA	Amino acid sequence. Enter a character string or vector of integers from the table. Examples: `'ARN'` or `[1 2 3]`. You can also enter a structure with the field `Sequence`.
ChartValue	Property to select a type of plot. Enter either `'pie'` or `'bar'`.
OthersValue	Property to control the counting of ambiguous characters individually. Enter either `'full'` or `'bundle'`(default).
StructureValue	Property to control blocking the unknown characters warning and to not count unknown characters.

Description

Amino = `aacount(`*SeqAA*`)` counts the type and number of amino acids in an amino acid sequence (*SeqAA*) and returns the counts in a 1-by-1 structure (*Amino*) with fields for the standard 20 amino acids (`A R N D C Q E G H I L K M F P S T W Y V`).

- If a sequence contains amino acids with ambiguous characters (`B`, `Z`, `X`), the stop character (`*`), or gaps indicated with a hyphen (`-`), the field `Others` is added to the structure and a warning message is displayed.

```
Warning: Symbols other than the standard 20 amino acids
appear in the sequence.
```

- If a sequence contains any characters other than the 20 standard amino acids, ambiguous characters, stop, and gap characters, the characters are counted in the field `Others` and a warning message is displayed.

  ```
  Warning: Sequence contains unknown characters. These will
  be ignored.
  ```

- If the property `Others = 'full'` , this function lists the ambiguous characters separately, asterisks are counted in a new field (`Stop`), and hyphens are counted in a new field (`Gap`).

`aacount(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs:

`aacount(..., 'Chart', ChartValue)` creates a chart showing the relative proportions of the amino acids.

`aacount(..., 'Others', OthersValue)`, when *OthersValue* is `'full''`, counts the ambiguous amino acid characters individually instead of adding them together in the field `Others`.

`aacount(..., 'Structure', StructureValue)`, when *StructureValue* is `'full'`, blocks the unknown characters warning and ignores counting unknown characters.

- `aacount(SeqAA)` — Display 20 amino acids, and only if there are ambiguous and unknown characters, add an `Others` field with the counts.
- `aacount(SeqAA, 'Others', 'full')` — Display 20 amino acids, 3 ambiguous amino acids, stops, gaps, and only if there are unknown characters, add an `Others` field with the unknown counts.
- `aacount(SeqAA, 'Structure', 'full')` — Display 20 amino acids and always display an `Others` field. If there are ambiguous and unknown characters, add counts to the `Others` field; otherwise display `0`.

- `aacount(SeqAA, 'Others', 'full', 'Structure', 'full')` — Display 20 amino acids, 3 ambiguous amino acids, stops, gaps, and `Others` field. If there are unknown characters, add counts to the `Others` field otherwise display `0`.

Examples

1 Create a sequence.

```
Seq =  aacount('MATLAB')
```

2 Count the amino acids in the sequence.

```
AA =  aacount(Seq)

Warning: Symbols other than the standard 20 amino acids appear
in the sequence.
AA =
     A: 2
     R: 0
     N: 0
     D: 0
     C: 0
     Q: 0
     E: 0
     G: 0
     H: 0
     I: 0
     L: 1
     K: 0
     M: 1
     F: 0
     P: 0
     S: 0
     T: 1
     W: 0
     Y: 0
     V: 0
Others: 1
```

3 Get the count for alanine (A) residues.

```
AA.A
ans =
      2
```

See Also

Bioinformatics Toolbox functions `aminolookup`, `atomiccomp`, `basecount`, `codoncount`, `dimercount`, `isoelectric`, `molweight`, `proteinplot`, `seqtool`

Purpose

Perform rank invariant set normalization on probe intensities from multiple Affymetrix CEL or DAT files

Syntax

```
NormData = affyinvarsetnorm(Data)
[NormData, MedStructure] = affyinvarsetnorm(Data)
... affyinvarsetnorm(..., 'Baseline', BaselineValue, ...)
... affyinvarsetnorm(..., 'Thresholds',
ThresholdsValue, ...)
... affyinvarsetnorm(..., 'StopPrctile',
StopPrctileValue, ...)
... affyinvarsetnorm(..., 'RayPrctile',
RayPrctileValue, ...)
... affyinvarsetnorm(..., 'Method', MethodValue, ...)
... affyinvarsetnorm(..., 'Showplot', ShowplotValue, ...)
```

Arguments

Data	Matrix of intensity values where each row corresponds to a perfect match (PM) probe and each column corresponds to an Affymetrix CEL or DAT file. (Each CEL or DAT file is generated from a separate chip. All chips should be of the same type.)
MedStructure	Structure of each column's intensity median before and after normalization, and the index of the column chosen as the baseline.
BaselineValue	Property to control the selection of the column index *N* from *Data* to be used as the baseline column. Default is the column index whose median intensity is the median of all the columns.

ThresholdsValue	Property to set the thresholds for the lowest average rank and the highest average rank, which are used to determine the invariant set. The rank invariant set is a set of data points whose proportional rank difference is smaller than a given threshold. The threshold for each data point is determined by interpolating between the threshold for the lowest average rank and the threshold for the highest average rank. Select these two thresholds empirically to limit the spread of the invariant set, but allow enough data points to determine the normalization relationship. `ThresholdsValue` is a 1-by-2 vector [*LT*, *HT*] where *LT* is the threshold for the lowest average rank and *HT* is threshold for the highest average rank. Values must be between `0` and `1`. Default is [`0.05, 0.005`].
StopPrctileValue	Property to stop the iteration process when the number of data points in the invariant set reaches *N* percent of the total number of data points. Default is `1`. **Note** If you do not use this property, the iteration process continues until no more data points are eliminated.
RayPrctileValue	Property to select the *N* percentage of the highest ranked invariant set of data points to fit a straight line through, while the remaining data points are fitted to a running median curve. The final running median curve is a piece-wise linear curve. Default is `1.5`.

MethodValue	Property to select the smoothing method used to normalize the data. Enter `'lowess'` or `'runmedian'`. Default is `'lowess'`.
ShowplotValue	Property to control the plotting of two pairs of scatter plots (before and after normalization). The first pair plots baseline data versus data from a specified column (chip) from the matrix *Data*. The second is a pair of M-A scatter plots, which plots M (ratio between baseline and sample) versus A (the average of the baseline and sample). Enter either `'all'` (plot a pair of scatter plots for each column or chip) or specify a subset of columns (chips) by entering the column number(s) or a range of numbers. For example: • `..., 'Showplot', 3, ...)` plots data from column 3. • `..., 'Showplot', [3,5,7], ...)` plots data from columns 3, 5, and 7. • `...  , 'Showplot', 3:9, ...)` plots data from columns 3 to 9.

Description

NormData = `affyinvarsetnorm(`*Data*`)` normalizes the values in each column (chip) of probe intensities in *Data* to a baseline reference, using the invariant set method. *NormData* is a matrix of normalized probe intensities from *Data*.

Specifically, `affyinvarsetnorm`:

- Selects a baseline index, typically the column whose median intensity is the median of all the columns.

- For each column, determines the proportional rank difference (*prd*) for each pair of ranks, *RankX* and *RankY*, from the sample column and the baseline reference.

  prd = abs(*RankX* - *RankY*)

- For each column, determines the invariant set of data points by selecting data points whose proportional rank differences (*prd*) are below *threshold*, which is a predetermined threshold for a given data point (defined by the `ThresholdsValue` property). It repeats the process until either no more data points are eliminated, or a predetermined percentage of data points is reached.

  The invariant set is data points with a *prd* < *threshold*.

- For each column, uses the invariant set of data points to calculate the lowess or running median smoothing curve, which is used to normalize the data in that column.

`[NormData, MedStructure] = affyinvarsetnorm(Data)` also returns a structure of the index of the column chosen as the baseline and each column's intensity median before and after normalization.

Note If `Data` contains NaN values, then `NormData` will also contain NaN values at the corresponding positions.

`... affyinvarsetnorm(..., 'PropertyName', PropertyValue, ...)` defines optional properties that use property name/value pairs in any order. These property name/value pairs are as follows:

`... affyinvarsetnorm(..., 'Baseline', BaselineValue, ...)` lets you select the column index `N` from `Data` to be the baseline column. Default is the index of the column whose median intensity is the median of all the columns.

... affyinvarsetnorm(..., 'Thresholds', *ThresholdsValue*, ...) sets the thresholds for the lowest average rank and the highest average rank, which are used to determine the invariant set. The rank invariant set is a set of data points whose proportional rank difference is smaller than a given threshold. The threshold for each data point is determined by interpolating between the threshold for the lowest average rank and the threshold for the highest average rank. Select these two thresholds empirically to limit the spread of the invariant set, but allow enough data points to determine the normalization relationship.

ThresholdsValue is a 1-by-2 vector [*LT, HT*] where *LT* is the threshold for the lowest average rank and *HT* is threshold for the highest average rank. Values must be between 0 and 1. Default is [0.05, 0.005].

... affyinvarsetnorm(..., 'StopPrctile', *StopPrctileValue*, ...) stops the iteration process when the number of data points in the invariant set reaches *N* percent of the total number of data points. Default is 1.

Note If you do not use this property, the iteration process continues until no more data points are eliminated.

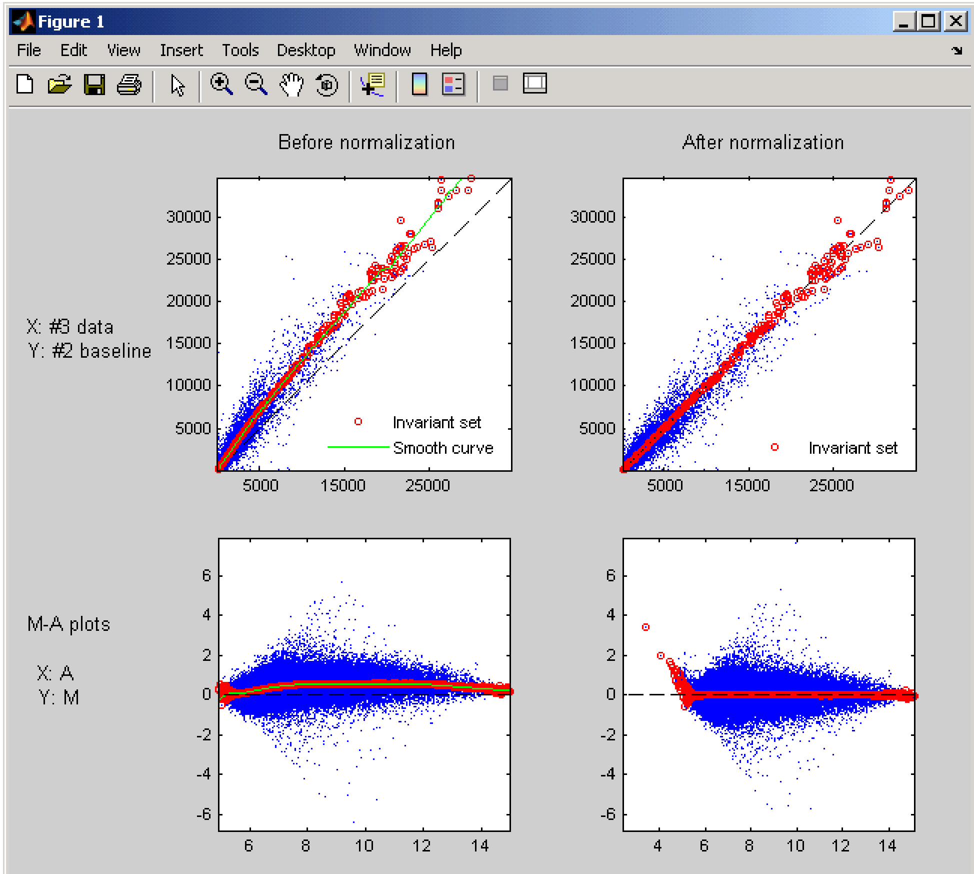
... affyinvarsetnorm(..., 'RayPrctile', *RayPrctileValue*, ...) selects the *N* percentage of the highest ranked invariant set of data points to fit a straight line through, while the remaining data points are fitted to a running median curve. The final running median curve is a piece-wise linear curve. Default is 1.5.

... affyinvarsetnorm(..., 'Method', *MethodValue*, ...) selects the smoothing method for normalizing the data. When *MethodValue* is 'lowess', affyinvarsetnorm uses the lowess method. When *MethodValue* is 'runmedian', affyinvarsetnorm uses the running median method. Default is 'lowess'.

... affyinvarsetnorm(..., 'Showplot', *ShowplotValue*, ...) plots two pairs of scatter plots (before and after normalization). The first pair plots baseline data versus data from a specified column (chip) from the matrix *Data*. The second is a pair of M-A scatter plots, which plots M (ratio between baseline and sample) versus A (the average of the baseline and sample). When *ShowplotValue* is `'all'`, `affyinvarsetnorm` plots a pair of scatter plots for each column or chip. When *ShowplotValue* is a number(s) or range of numbers, `affyinvarsetnorm` plots a pair of scatter plots for the indicated column numbers (chips).

For example:

- `..., 'Showplot', 3)` plots the data from column 3 of *Data*.
- `..., 'Showplot', [3,5,7])` plots the data from columns 3, 5, and 7 of *Data*.
- `..., 'Showplot', 3:9)` plots the data from columns 3 to 9 of *Data*.



Examples

1 Load a MAT file, included with Bioinformatics Toolbox, which contains Affymetrix data variables, including `pmMatrix`, a matrix of PM probe intensity values from multiple CEL files.

```
load prostatecancerrawdata
```

2 Normalize the data in `pmMatrix`, using the `affyinvarsetnorm` function.

```
NormMatrix = affyinvarsetnorm(pmMatrix);
```

The `prostatecancerrawdata.mat` file used in the previous example contains data from Best et al., 2005.

References

[1] Li, C., and Wong, W.H. (2001). Model-based analysis of oligonucleotide arrays: model validation, design issues and standard error application. Genome Biology *2(8)*: research0032.1-0032.11.

[2] http://biosun1.harvard.edu/complab/dchip/normalizing%20arrays.htm#isn

[3] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823-6834.

See Also

`affyread`, `celintensityread`, `mainvarsetnorm`, `malowess`, `manorm`, `quantilenorm`, `rmabackadj`, `rmasummary`

Purpose

Compute Affymetrix probe affinities from their sequences and MM probe intensities

Syntax

```
[AffinPM, AffinMM] = affyprobeaffinities(SequenceMatrix,
   MMIntensity)
[AffinPM, AffinMM,
   BaseProf] = affyprobeaffinities(SequenceMatrix,
   MMIntensity)
[AffinPM, AffinMM, BaseProf,
   Stats] = affyprobeaffinities(SequenceMatrix, MMIntensity)
... = affyprobeaffinities(SequenceMatrix, MMIntensity,
...'ProbeIndices', ProbeIndicesValue, ...)
... = affyprobeaffinities(SequenceMatrix, MMIntensity,
   ...'Showplot', ShowplotValue, ...)
```

Arguments

SequenceMatrix

An N-by-25 matrix of sequence information for the perfect match (PM) probes on an Affymetrix GeneChip array, where N is the number of probes on the array. Each row corresponds to a probe, and each column corresponds to one of the 25 sequence positions. Nucleotides in the sequences are represented by one of the following integers:

- `0` — None
- `1` — A
- `2` — C
- `3` — G
- `4` — T

Tip You can use the `affyprobeseqread` function to generate this matrix. If you have this sequence information in letter representation, you can convert it to integer representation using the `nt2int` function.

MMIntensity

Column vector containing mismatch (MM) probe intensities from a CEL file, generated from a single Affymetrix GeneChip array. Each row corresponds to a probe.

Tip You can extract this column vector from the `MMIntensities` matrix returned by the `celintensityread` function.

ProbeIndicesValue	Column vector containing probe indexing information. Probes within a probe set are numbered 0 through *N* - 1, where *N* is the number of probes in the probe set. **Tip** You can use the `affyprobeseqread` function to generate this column vector.
ShowplotValue	Controls the display of a plot showing the affinity values of each of the four bases (A, C, G, and T) for each of the 25 sequence positions, for all probes on the Affymetrix GeneChip array. Choices are `true` or `false` (default).

Return Values

AffinPM	Column vector of PM probe affinities, computed from their probe sequences and MM probe intensities.
AffinMM	Column vector of MM probe affinities, computed from their probe sequences and MM probe intensities.

Description

`[`*`AffinPM`*`, `*`AffinMM`*`] = affyprobeaffinities(`*`SequenceMatrix`*`, `*`MMIntensity`*`)` returns a column vector of PM probe affinities and a column vector of MM probe affinities, computed from their probe sequences and MM probe intensities. Each row in *`AffinPM`* and *`AffinMM`* corresponds to a probe. NaN is returned for probes with no sequence information. Each probe affinity is the sum of position-dependent base affinities. For a given base type, the positional effect is modeled as a polynomial of degree 3.

`[`*`AffinPM`*`, `*`AffinMM`*`, `*`BaseProf`*`] = affyprobeaffinities(`*`SequenceMatrix`*`, `*`MMIntensity`*`)` also estimates affinity coefficients using multiple linear regression. It returns *BaseProf*, a 4-by-4 matrix containing the four parameters for a polynomial of degree 3, for each base, A, C, G, and T. Each row corresponds to a base, and each column corresponds to a parameter. These values are estimated from the probe sequences and intensities, and represent all probes on an Affymetrix GeneChip array.

`[AffinPM, AffinMM, BaseProf, Stats] = affyprobeaffinities(SequenceMatrix, MMIntensity)` also returns *Stats*, a row vector containing four statistics in the following order:

- R-square statistic
- F statistic
- p value
- error variance

`... = affyprobeaffinities(SequenceMatrix, MMIntensity, ...'PropertyName', PropertyValue, ...)` calls `affyprobeaffinities` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = affyprobeaffinities(SequenceMatrix, MMIntensity, ...'ProbeIndices', ProbeIndicesValue, ...)` uses probe indices to normalize the probe intensities with the median of their probe set intensities.

Tip Use of the `ProbeIndices` property is recommended only if your *MMIntensity* data are not from a nonspecific binding experiment.

`... = affyprobeaffinities(SequenceMatrix, MMIntensity, ...'Showplot', ShowplotValue, ...)` controls the display of a plot of the probe affinity base profile. Choices are `true` or `false` (default).

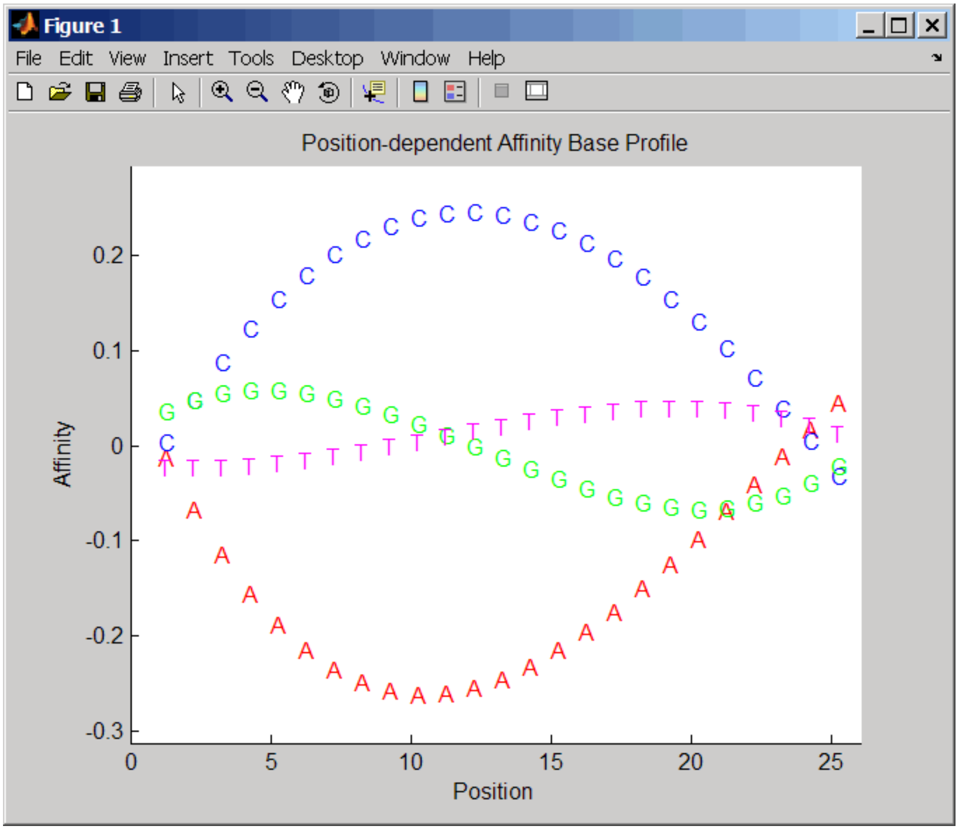
Examples

1. Load the MAT file, included with Bioinformatics Toolbox, that contains Affymetrix data from a prostate cancer study. The variables in the MAT file include `seqMatrix`, a matrix containing sequence information for PM probes, `mmMatrix`, a matrix containing MM probe intensity values, and `probeIndices`, a column vector containing probe indexing information.

```
load prostatecancerrawdata
```

2. Compute the Affymetrix PM and MM probe affinities from their sequences and MM probe intensities, and also plot the affinity values of each of the four bases (A, C, G, and T) for each of the 25 sequence positions, for all probes on the Affymetrix GeneChip array.

```
[apm, amm] = affyprobeaffinities(seqMatrix, mmMatrix(:,1),...
             'ProbeIndices', probeIndices, 'showplot', true);
```



The `prostatecancerrawdata.mat` file used in this example contains data from Best et al., 2005.

References

[1] Naef, F., and Magnasco, M.O. (2003). Solving the Riddle of the Bright Mismatches: Labeling and Effective Binding in Oligonucleotide Arrays. Physical Review E *68*, 011906.

[2] Wu, Z., Irizarry, R.A., Gentleman, R., Murillo, F.M. and Spencer, F. (2004). A Model Based Background Adjustment for Oligonucleotide

Expression Arrays. Journal of the American Statistical Association *99(468)*, 909–917.

[3] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

See Also

Bioinformatics Toolbox functions: `affyprobeseqread`, `affyread`, `celintensityread`, `probelibraryinfo`

Purpose

Read data file containing probe sequence information for Affymetrix GeneChip array

Syntax

```
Struct = affyprobeseqread(SeqFile, CDFFile)
Struct = affyprobeseqread(SeqFile, CDFFile, ...'SeqPath',
SeqPathValue, ...)
Struct = affyprobeseqread(SeqFile, CDFFile, ...'CDFPath',
   CDFPathValue, ...)
Struct = affyprobeseqread(SeqFile, CDFFile, ...'SeqOnly',
   SeqOnlyValue, ...)
```

Arguments

`SeqFile` — String specifying a file name of a sequence file (tab-separated or FASTA) that contains the following information for a specific type of Affymetrix GeneChip array:

- Probe set IDs
- Probe *x*-coordinates
- Probe *y*-coordinates
- Probe sequences in each probe set
- Affymetrix GeneChip array type (FASTA file only)

The sequence file (tab-separated or FASTA) must be on the MATLAB search path or in the Current Directory (unless you use the `SeqPath` property). In a tab-separated file, each row represents a probe; in a FASTA file, each header represents a probe.

`CDFFile` — Either of the following:

- String specifying a file name of an Affymetrix CDF library file, which contains information that specifies which probe set each probe belongs to on a specific type of Affymetrix GeneChip array. The CDF library file must be on the MATLAB search path or in the MATLAB Current Directory (unless you use the `CDFPath` property).
- CDF structure, such as returned by the `affyread` function, which contains information that specifies which probe set each probe belongs to on a specific type of Affymetrix GeneChip array.

Caution Make sure that *`SeqFile`* and *`CDFFile`* contain information for the same type of Affymetrix GeneChip array.

SeqPathValue	String specifying a directory or path and directory where *SeqFile* is stored.
CDFPathValue	String specifying a directory or path and directory where *CDFFile* is stored.
SeqOnlyValue	Controls the return of a structure, *Struct*, with only one field, `SequenceMatrix`. Choices are `true` or `false` (default).

Return Values

Struct — MATLAB structure containing the following fields:

- `ProbeSetIDs`
- `ProbeIndices`
- `SequenceMatrix`

Description

Struct = `affyprobeseqread(`*SeqFile*`,` *CDFFile*`)` reads the data from files *SeqFile* and *CDFFile*, and stores the data in the MATLAB structure *Struct*, which contains the following fields.

Field	Description
`ProbeSetIDs`	Cell array containing the probe set IDs from the Affymetrix CDF library file.

Field	Description
`ProbeIndices`	Column vector containing probe indexing information. Probes within a probe set are numbered 0 through *N* - 1, where *N* is the number of probes in the probe set.
`SequenceMatrix`	An *N*-by-25 matrix of sequence information for the perfect match (PM) probes on the Affymetrix GeneChip array, where *N* is the number of probes on the array. Each row corresponds to a probe, and each column corresponds to one of the 25 sequence positions. Nucleotides in the sequences are represented by one of the following integers: • `0` — None • `1` — A • `2` — C • `3` — G • `4` — T **Note** Probes without sequence information are represented in `SequenceMatrix` as a row containing all `0`s. **Tip** You can use the `int2nt` function to convert the nucleotide sequences in `SequenceMatrix` to letter representation.

`*Struct* = affyprobeseqread(*SeqFile*, *CDFFile*, ...'*PropertyName*', *PropertyValue*, ...)` calls `affyprobeseqread` with optional properties that use property name/property value pairs.

You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`Struct = affyprobeseqread(SeqFile, CDFFile, ...'SeqPath', SeqPathValue, ...)` lets you specify a path and directory where `SeqFile` is stored.

`Struct = affyprobeseqread(SeqFile, CDFFile, ...'CDFPath', CDFPathValue, ...)` lets you specify a path directory where `CDFFile` is stored.

`Struct = affyprobeseqread(SeqFile, CDFFile, ...'SeqOnly', SeqOnlyValue, ...)` controls the return of a structure, `Struct`, with only one field, `SequenceMatrix`. Choices are `true` or `false` (default).

Examples

1. Read the data from a FASTA file and associated CDF library file, assuming both are located on the MATLAB search path or in the Current Directory.

```
S1 = affyprobeseqread('HG-U95A_probe_fasta', 'HG_U95A.CDF');
```

2. Read the data from a tab-separated file and associated CDF structure, assuming the tab-separated file is located in the specified directory and the CDF structure is in your MATLAB Workspace.

```
S2 = affyprobeseqread('HG-U95A_probe_tab',hgu95aCDFStruct,...
     'seqpath','C:\Affymetrix\SequenceFiles\HGGenome');
```

3. Access the nucleotide sequences of the first probe set (rows 1 through 20) in the `SequenceMatrix` field of the `S2` structure.

```
seq = int2nt(S2.SequenceMatrix(1:20,:))
```

See Also

Bioinformatics Toolbox functions: `affyinvarsetnorm`, `affyread`, `celintensityread`, `int2nt`, `probelibraryinfo`, `probesetlink`, `probesetlookup`, `probesetplot`, `probesetvalues`

affyread

Purpose Read microarray data from Affymetrix GeneChip file (Windows 32)

Syntax

```
AffyStruct = affyread(File)
AffyStruct = affyread(File, LibraryPath)
```

Arguments

File — String specifying a file name or a path and file name of one of the following Affymetrix file types:

- **DAT** — Data file containing raw image data.
- **CEL** — Data file containing information about the expression levels of the individual probes.
- **CHP** — Data file containing information about probe sets.
- **EXP** — Data file containing information about experimental conditions and protocols.
- **CDF** — Library file containing information about which probes belong to which probe set.
- **GIN** — Library file containing information about the probe sets, such as the gene name with which the probe set is associated.

If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Directory.

LibraryPath — String specifying the path and directory where the library file (CDF or GIN) associated with `File` is stored.

Note This input argument is needed only if `File` is a CHP file.

Return Values

AffyStruct	MATLAB structure containing information from the Affymetrix data or library file.

Description

Note This function is supported on the Windows 32 platform only.

`AffyStruct = affyread(File)` reads *File*, an Affymetrix file, and creates *AffyStruct*, a MATLAB structure.

AffyStruct contains the following fields:

`AffyStruct = affyread(File, LibraryPath)` specifies the path and directory where the library file (CDF or GIN) associated with *File* is stored. Use this syntax only if *File* is a CHP file.

You can learn more about the Affymetrix GeneChip files and download sample files from:

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

Note Some Affymetrix sample data files (DAT, EXP, CEL, and CHP) are combined together in a DTT file. You must download and use the Affymetrix Data Transfer Tool to extract these files from the DTT file.

Caution

When using `affyread` to read a CHP file, the Affymetrix GDAC Runtime Libraries look for the associated CEL file in the directory that it was in when the CHP file was created. If the CEL file is not found, then `affyread` does not read probe set values in the CHP file.

If you encounter errors reading files, then check that the Affymetrix GDAC Runtime Libraries are correctly installed. You can reinstall the libraries by running the installer from Windows Explorer:

```
$MATLAB$\toolbox\bioinfo\microarray\lib\...
GdacFilesRuntimeInstall-v4.exe
```

Examples

The following example assumes that `Drosophila.CEL` and `Drosophila.dat` are stored on the MATLAB search path or in the MATLAB Current Directory. It also assumes that `Drosophila.chp` is stored on the MATLAB search path or in the MATLAB Current Directory, and that its associated library file is stored at D:\Affymetrix\LibFiles\DrosGenome1.

1 Read the contents of a CEL file into a MATLAB structure.

```
celStruct = affyread('Drosophila.CEL')
```

2 Display a spatial plot of the probe intensities.

```
maimage(celStruct, 'Intensity')
```

3 Read the contents of a DAT file into a MATLAB structure, and then display the raw image data.

```
datStruct = affyread('Drosophila.dat')
imagesc(datStruct.Image);
axis image;
```

4 Read the contents of a CHP file into a MATLAB structure, and then plot the probe values for a probe set. The CHP files require the library files. Your file may be in a different location than this example.

```
chpStruct = affyread('Drosophila.chp',...
            'D:\Affymetrix\LibFiles\DrosGenome1')
geneName = probesetlookup(chpStruct,'14317_at')
probesetplot(chpStruct,'142417_at');
```

See Also

Bioinformatics Toolbox functions: `agferead`, `celintensityread`, `gprread`, `probelibraryinfo`, `probesetlink`, `probesetlookup`, `probesetplot`, `probesetvalues`, `sptread`

Purpose

Read Agilent Feature Extraction Software file

Syntax

`AGFEData = agferead(File)`

Arguments

`File`	Microarray data file generated with the Agilent Feature Extraction Software.

Description

`AGFEData` `= agferead(`*`File`*`)` reads files generated with Feature Extraction Software from Agilent micoararry scanners and creates a structure (*`AGFEData`*) containing the following fields:

- `Header`
- `Stats`
- `Columns`
- `Rows`
- `Names`
- `IDs`
- `Data`
- `ColumnNames`
- `TextData`
- `TextColumnNames`

Feature Extraction Software takes an image from an Agilent microarray scanner and generates raw intensity data for each spot on the plate. For more information about this software, see a description on their Web site at

`http://www.chem.agilent.com/scripts/pds.asp?lpage=2547`

Examples

1. Read in a sample Agilent Feature Extraction Software file. Note that the file `fe_sample.txt` is not provided with Bioinformatics Toolbox.

```
agfeStruct = agferead('fe_sample.txt')
```

2 Plot the median foreground.

```
maimage(agfeStruct,'gMedianSignal');
maboxplot(agfeStruct,'gMedianSignal');
```

See Also

Bioinformatics Toolbox functions: `affyread`, `celintensityread`, `galread`, `geosoftread`, `gprread`, `imageneread`, `magetfield`, `sptread`

Purpose

Find amino acid codes, integers, abbreviations, names, and codons

Syntax

```
aminolookup
aminolookup(SeqAA)
aminolookup('Code', CodeValue)
aminolookup('Integer', IntegerValue)
aminolookup('Abbreviation', AbbreviationValue)
aminolookup('Name', NameValue)
```

Arguments

SeqAA	Character string of single-letter codes or three-letter abbreviations representing an amino acid sequence. See the Amino Acid Lookup Table on page 2-42 for valid codes and abbreviations.
CodeValue	String specifying a single-letter representing an amino acid. See the Amino Acid Lookup Table on page 2-42 for valid single-letter codes.
IntegerValue	Single integer representing an amino acid. See the Amino Acid Lookup Table on page 2-42 for valid integers.
AbbreviationValue	String specifying a three-letter abbreviation representing an amino acid. See the Amino Acid Lookup Table on page 2-42 for valid three-letter abbreviations.
NameValue	String specifying an amino acid name. See the Amino Acid Lookup Table on page 2-42 for valid amino acid names.

Amino Acid Lookup Table

Code	Integer	Abbreviation	Name	Codons
A	1	Ala	Alanine	GCU GCC GCA GCG
R	2	Arg	Arginine	CGU CGC CGA CGG AGA AGG
N	3	Asn	Asparagine	AAU AAC
D	4	Asp	Aspartic acid (Aspartate)	GAU GAC
C	5	Cys	Cysteine	UGU UGC
Q	6	Gln	Glutamine	CAA CAG
E	7	Glu	Glutamic acid (Glutamate)	GAA GAG
G	8	Gly	Glycine	GGU GGC GGA GGG
H	9	His	Histidine	CAU CAC
I	10	Ile	Isoleucine	AUU AUC AUA
L	11	Leu	Leucine	UUA UUG CUU CUC CUA CUG
K	12	Lys	Lysine	AAA AAG
M	13	Met	Methionine	AUG
F	14	Phe	Phenylalanine	UUU UUC
P	15	Pro	Proline	CCU CCC CCA CCG
S	16	Ser	Serine	UCU UCC UCA UCG AGU AGC
T	17	Thr	Threonine	ACU ACC ACA ACG
W	18	Trp	Tryptophan	UGG
Y	19	Tyr	Tyrosine	UAU UAC

Code	Integer	Abbreviation	Name	Codons
V	20	Val	Valine	GUU GUC GUA GUG
B	21	Asx	Asparagine or Aspartic acid	AAU AAC GAU GAC
Z	22	Glx	Glutamine or Glutamic acid	CAA CAG GAA GAG
X	23	Xaa	Any amino acid	All codons
*	24	END	Termination (translation stop)	UAA UAG UGA
-	25	GAP	Gap of unknown length	- - -

Description

`aminolookup` displays a table of amino acid codes, integers, abbreviations, names, and codons.

`aminolookup(`*`SeqAA`*`)` converts between three-letter abbreviations and single-letter codes for an amino acid sequence. If the input is a character string of three-letter abbreviations, then the output is a character string of the corresponding single-letter codes. If the input is a character string of single-letter codes, then the output is a character string of three-letter abbreviations.

If you enter one of the ambiguous single-letter codes `B`, `Z`, or `X`, this function displays the corresponding abbreviation for the ambiguous amino acid character.

```
aminolookup('abc')

ans =

AlaAsxCys
```

`aminolookup('Code', CodeValue)` displays the corresponding amino acid three-letter abbreviation and name.

`aminolookup('Integer', IntegerValue)` displays the corresponding amino acid single-letter code, three-letter abbreviation, and name.

`aminolookup('Abbreviation', AbbreviationValue)` displays the corresponding amino acid single-letter code and name.

`aminolookup('Name', NameValue)` displays the corresponding amino acid single-letter code and three-letter abbreviation.

Examples

1 Convert an amino acid sequence in single-letter codes to the corresponding three-letter abbreviations.

```
aminolookup('MWKQAEDIRDIYDF')

ans =

MetTrpLysGlnAlaGluAspIleArgAspIleTyrAspPhe
```

2 Convert an amino acid sequence in three-letter abbreviations to the corresponding single-letter codes.

```
aminolookup('MetTrpLysGlnAlaGluAspIleArgAspIleTyrAspPhe')

ans =

MWKQAEDIRDIYDF
```

3 Display the three-letter abbreviation and name for the amino acid corresponding to the single-letter code `R`.

```
aminolookup('code', 'R')

ans =

Arg Arginine
```

4 Display the single-letter code, three-letter abbreviation, and name for the amino acid corresponding to the integer `1`.

```
aminolookup('integer', 1)

ans =

A Ala Alanine
```

5 Display the single-letter code and name for the amino acid corresponding to the three-letter abbreviation `asn`.

```
aminolookup('abbreviation', 'asn')

ans =

N Asparagine
```

6 Display the single-letter code and three-letter abbreviation for the amino acid proline.

```
aminolookup('Name','proline')

ans =

P Pro
```

See Also

Bioinformatics Toolbox functions: `aa2int`, `aacount`, `geneticcode`, `int2aa`, `nt2aa`, `revgeneticcode`

atomiccomp

Purpose Calculate atomic composition of protein

Syntax `NumberAtoms = atomiccomp(SeqAA)`

Arguments

SeqAA	Amino acid sequence. Enter a character string or vector of integers from the table . You can also enter a structure with the field `Sequence`.

Description *NumberAtoms* = `atomiccomp(`*SeqAA*`)` counts the type and number of atoms in an amino acid sequence (*SeqAA*) and returns the counts in a `1`-by-`1` structure (*NumberAtoms*) with fields `C`, `H`, `N`, `O`, and `S`.

Examples

1 Get an amino acid sequence from the NCBI Genpept Database.

```
rhodopsin = getgenpept('NP_000530');
```

2 Count the atoms in a sequence.

```
rhodopsinAC = atomiccomp(rhodopsin)

rhodopsinAC =

    C: 1814
    H: 2725
    N: 423
    O: 477
    S: 25
```

3 Retrieve the number of carbon atoms in the sequence.

```
rhodopsinAC.C

ans =

        1814
```

See Also Bioinformatics Toolbox functions `aacount`, `molweight`, `proteinplot`

basecount

Purpose Count nucleotides in sequence

Syntax

```
NumberBases = basecount(SeqNT)
basecount(..., 'PropertyName', PropertyValue,...)
basecount(..., 'Chart', ChartValue)
basecount(..., 'Others', OthersValue)
basecount(..., 'Structure', StructureValue),
```

Arguments

SeqNT	Nucleotide sequence. Enter a character string with the letters A, T, U, C, and G. The count for U characters is included with the count for T characters. . You can also enter a structure with the field Sequence.
ChartValue	Property to select a type of plot. Enter either 'pie' or 'bar'.
OthersValue	Property to control counting ambiguous characters individually. Enter either full' or 'bundle' (default).

Description *NumberBases* = basecount(*SeqNT*) counts the number of bases in a nucleotide sequence (SeqNT) and returns the base counts in a 1-by-1 structure (Bases) with the fields A, C, G, T.

- For sequences with the character U, the number of U characters is added to the number of T characters.
- If a sequence contains ambiguous nucleotide characters (R, Y, K, M, S, W, B, D, H, V, N), or gaps indicated with a hyphen (-), this function creates a field Others and displays a warning message.

```
Warning: Ambiguous symbols 'symbol list' appear
in the sequence.
These will be in Others.
```

- If a sequence contains undefined nucleotide characters (`E F H I J L O P Q X Z`), the characters are counted in the field `Others` and a warning message is displayed.

  ```
  Warning: Unknown symbols 'symbol list' appear
  in the sequence.
  These will be ignored.
  ```

- If the property `Others = 'full'`, ambiguous characters are listed separately and hyphens are counted in a new field (`Gaps`).

`basecount(..., '`*`PropertyName`*`', `*`PropertyValue`*`,...)` defines optional properties using property name/value pairs:

`basecount(..., 'Chart', `*`ChartValue`*`)` creates a chart showing the relative proportions of the nucleotides.

`basecount(..., 'Others', `*`OthersValue`*`)`, when *`OthersValue`* is `'full'`, counts all the ambiguous nucleotide symbols individually instead of bundling them together into the `Others` field of the output structure.

`basecount(..., 'Structure', `*`StructureValue`*`)`, when *`StructureValue`* is `'full'`, blocks the unknown characters warning and ignores counting unknown characters.

- `basecount(SeqNT)` — Display four nucleotides, and only if there are ambiguous and unknown characters, add an `Others` field with the counts.
- `basecount(SeqNT, 'Others', 'full')` — Display four nucleotides, 11 ambiguous nucleotides, gaps, and only if there are unknown characters, add an `Others` field with the unknown counts.
- `basecount(SeqNT, 'Structure', 'full')` — Display four nucleotides and always display an `Others` field. If there are ambiguous and unknown characters, add counts to the `Others` field; otherwise display `0`.

- `basecount(SeqNT, 'Others', 'full', 'Structure', 'full')` — Display 4 nucleotides, 11 ambiguous nucleotides, gaps, and the `Others` field. If there are unknown characters, add counts to the `Others` field; otherwise display `0`.

Examples

1 Count the number of bases in a DNA sequence.

```
Bases = basecount('TAGCTGGCCAAGCGAGCTTG')

Bases =
    A: 4
    C: 5
    G: 7
    T: 4
```

2 Get the count for adenosine (A) bases.

```
Bases.A

ans =
    4
```

3 Count the bases in a DNA sequence with ambiguous characters.

```
basecount('ABCDGGCCAAGCGAGCTTG','Others','full')

ans =
    A: 4
    C: 5
    G: 6
    T: 2
    R: 0
    Y: 0
    K: 0
    M: 0
    S: 0
    W: 0
    B: 1
```

```
   D: 1
   H: 0
   V: 0
   N: 0
Gaps: 0
```

See Also

Bioinformatics Toolbox functions `aacount`, `baselookup`, `codoncount`, `cpgisland`, `dimercount`, `nmercount`, `ntdensity`, `seqtool`

baselookup

Purpose

Nucleotide codes, abbreviations, and names

Syntax

```
baselookup('Complement', SeqNT)
baselookup('Code', CodeValue)
baselookup('Integer', IntegerValue)
baselookup('Name', NameValue)
```

Arguments

SeqNT	Nucleotide sequence. Enter a character string of single-letter codes from the Nucleotide Lookup Table below. In addition to a single nucleotide sequence, *SeqNT* can be a cell array of sequences, or a two-dimensional character array of sequences. The complement for each sequence is determined independently.
CodeValue	Nucleotide letter code. Enter a single character from the Nucleotide Lookup Table below. `Code` can also be a cell array or a two-dimensional character array.
IntegerValue	Nucleotide integer. Enter an integer from the Nucleotide Lookup Table below. Integers are arbitrarily assigned to IUB/IUPAC letters.
NameValue	Nucleotide name. Enter a nucleotide name from the Nucleotide Lookup Table below. *NameValue* can also be a single name, a cell array, or a two-dimensional character array.

Nucleotide Lookup Table

Code	Integer	Base Name	Meaning	Complement
A	1	Adenine	A	T
C	2	Cytosine	C	G

Code	Integer	Base Name	Meaning	Complement
G	3	Guanine	G	C
T	4	Thymine	T	A
U	4	Uracil	U	A
R	5	(Purine)	G|A	Y
Y	6	(Pyrimidine)	T|C	R
K	7	(Keto)	G|T	M
M	8	(Amino)	A|C	K
S	9	Strong interaction (3 H bonds)	G|C	S
W	10	Weak interaction (2 H bonds)	A|T	W
B	11	Not A	G|T|C	V
D	12	Not C	G|A|T	H
H	13	Not G	A|T|C	D
V	14	Not T or U	G|A|C	B
N,X	15	Any nucleotide	G|A|T|C	N
-	16	Gap of indeterminate length	Gap	-

Description

`baselookup('Complement', SeqNT)` displays the complementary nucleotide sequence.

`baselookup('Code', CodeValue)` displays the corresponding letter code, meaning, and name. For ambiguous nucleotide letters (`R Y K M S W B D H V N X`), the name is replace by a descriptive name.

`baselookup('Integer', IntegerValue)` displays the corresponding letter code, meaning, and nucleotide name.

`baselookup('Name', NameValue)` displays the corresponding letter code and meaning.

Examples

```
baselookup('Complement', 'TAGCTGRCCAAGGCCAAGCGAGCTTN')

baselookup('Name','cytosine')
```

See Also

Bioinformatics Toolbox functions `basecount`, `codoncount`, `dimercount`, `geneticcode`, `nt2aa`, `nt2int`, `revgeneticcode`, `seqtool`

Purpose

Create biograph object

Syntax

```
BGobj = biograph(CMatrix)
BGobj = biograph(CMatrix, NodeIDs)
BGobj = biograph(CMatrix, NodeIDs, ...'ID', IDValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'Label', LabelValue,
   ...)
BGobj = biograph(CMatrix, NodeIDs, ...'Description',
   DescriptionValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'LayoutType',
   LayoutTypeValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'EdgeType',
   EdgeTypeValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'Scale', ScaleValue,
   ...)
BGobj = biograph(CMatrix, NodeIDs, ...'LayoutScale',
   LayoutScaleValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'EdgeTextColor',
   EdgeTextColorValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'EdgeFontSize',
   EdgeFontSizeValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'ShowArrows',
   ShowArrowsValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'ArrowSize',
   ArrowSizeValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'ShowWeights',
   ShowWeightsValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'ShowTextInNodes',
   ShowTextInNodesValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'NodeAutoSize',
   NodeAutoSizeValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'NodeCallback',
   NodeCallbackValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'EdgeCallback',
   EdgeCallbackValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'CustomNodeDrawFcn',
   CustomNodeDrawFcnValue, ...)
```

Arguments

CMatrix	Full or sparse square matrix that acts as a connection matrix. That is, a value of `1` indicates a connection between nodes while a `0` indicates no connection. The number of rows/columns is equal to the number of nodes.
NodeIDs	Node identification strings. Enter any of the following: • Cell array of strings with the number of strings equal to the number of rows or columns in the connection matrix *CMatrix*. Each string must be unique. • Character array with the number of rows equal to the number of nodes. Each row in the array must be unique. • String with the number of characters equal to the number of nodes. Each character must be unique. Default values are the row or column numbers. **Note** You must specify *NodeIDs* if you want to specify property name/value pairs. Set *NodeIDs* to `[]` to use the default values of the row/column numbers.
IDValue	String to identify the biograph object. Default is `''`. (This information is for bookkeeping purposes only.)

LabelValue	String to label the biograph object. Default is `''`. (This information is for bookkeeping purposes only.)
DescriptionValue	String that describes the biograph object. Default is `''`. (This information is for bookkeeping purposes only.)
LayoutTypeValue	String that specifies the algorithm for the layout engine. Choices are: • `'hierarchical'` (default) • `'equilibrium'` • `'radial'`
EdgeTypeValue	String that specifies how edges display. Choices are: • `'straight'` • `'curved'` (default) • `'segmented'` **Note** Curved or segmented edges occur only when necessary to avoid obstruction by nodes. Biograph objects with `LayoutType` equal to `'equilibrium'` or `'radial'` cannot produce curved or segmented edges.
ScaleValue	Positive number that post-scales the node coordinates. Default is `1`.
LayoutScaleValue	Positive number that scales the size of the nodes before calling the layout engine. Default is `1`.

EdgeTextColorValue	Three-element numeric vector of RGB values. Default is `[0, 0, 0]`, which defines black.
EdgeFontSizeValue	Positive number that sets the size of the edge font in points. Default is `8`.
ShowArrowsValue	Controls the display of arrows for the edges. Choices are `'on'` (default) or `'off'`.
ArrowSizeValue	Positive number that sets the size of the arrows in points. Default is `8`.
ShowWeightsValue	Controls the display of text indicating the weight of the edges. Choices are `'on'` (default) or `'off'`.
ShowTextInNodesValue	String that specifies the node property used to label nodes when you display a biograph object using the `view` method. Choices are: • `'Label'` — Uses the `Label` property of the node object (default). • `'ID'` — Uses the `ID` property of the node object. • `'None'`

NodeAutoSizeValue	Controls precalculating the node size before calling the layout engine. Choices are `'on'` (default) or `'off'`.
NodeCallbackValue	User callback for all nodes. Enter the name of a function, a function handle, or a cell array with multiple function handles. After using the `view` function to display the biograph in the Biograph Viewer, you can double-click a node to activate the first callback, or right-click and select a callback to activate. Default is `@(node) inspect(node)`, which displays the Property Inspector dialog box.
EdgeCallbackValue	User callback for all edges. Enter the name of a function, a function handle, or a cell array with multiple function handles. After using the `view` function to display the biograph in the Biograph Viewer, you can double-click an edge to activate the first callback, or right-click and select a callback to activate. Default is `@(edge) inspect(edge)`, which displays the Property Inspector dialog box.
CustomNodeDrawFcnValue	Function handle to customized function to draw nodes. Default is `[]`.

Description

`BGobj = biograph(CMatrix)` creates a biograph object, *BGobj*, using a connection matrix, *CMatrix*. All nondiagonal and positive entries in the connection matrix, *CMatrix*, indicate connected nodes, rows represent the source nodes, and columns represent the sink nodes.

`BGobj = biograph(CMatrix, NodeIDs)` specifies the node identification strings. *NodeIDs* can be:

- Cell array of strings with the number of strings equal to the number of rows or columns in the connection matrix *CMatrix*. Each string must be unique.
- Character array with the number of rows equal to the number of nodes. Each row in the array must be unique.
- String with the number of characters equal to the number of nodes. Each character must be unique.

Default values are the row or column numbers.

Note If you want to specify property name/value pairs, you must specify *NodeIDs*. Set *NodeIDs* to `[]` to use the default values of the row/column numbers.

`BGobj = biograph(..., 'PropertyName', PropertyValue, ...)` calls `biograph` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`BGobj = biograph(CMatrix, NodeIDs, ...'ID', IDValue, ...)` specifies an ID for the biograph object. Default is `''`. (This information is for bookkeeping purposes only.)

`BGobj = biograph(CMatrix, NodeIDs, ...'Label', LabelValue, ...)` specifies a label for the biograph object. Default is `''`. (This information is for bookkeeping purposes only.)

`BGobj = biograph(CMatrix, NodeIDs, ...'Description', DescriptionValue, ...)` specifies a description of the biograph object. Default is `''`. (This information is for bookkeeping purposes only.)

`BGobj = biograph(CMatrix, NodeIDs, ...'LayoutType', LayoutTypeValue, ...)` specifies the algorithm for the layout engine.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'EdgeType', *EdgeTypeValue*, ...) specifies how edges display.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'Scale', *ScaleValue*, ...) post-scales the node coordinates. Default is 1.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'LayoutScale', *LayoutScaleValue*, ...) scales the size of the nodes before calling the layout engine. Default is 1.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'EdgeTextColor', *EdgeTextColorValue*, ...) specifies a three-element numeric vector of RGB values. Default is [0, 0, 0], which defines black.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'EdgeFontSize', *EdgeFontSizeValue*, ...) sets the size of the edge font in points. Default is 8.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'ShowArrows', *ShowArrowsValue*, ...) controls the display of arrows for the edges. Choices are 'on' (default) or 'off'.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'ArrowSize', *ArrowSizeValue*, ...) sets the size of the arrows in points. Default is 8.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'ShowWeights', *ShowWeightsValue*, ...) controls the display of text indicating the weight of the edges. Choices are 'on' (default) or 'off'.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'ShowTextInNodes', *ShowTextInNodesValue*, ...) specifies the node property used to label nodes when you display a biograph object using the view method.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'NodeAutoSize', *NodeAutoSizeValue*, ...) controls precalculating the node size before calling the layout engine. Choices are 'on' (default) or 'off'.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'NodeCallback', *NodeCallbackValue*, ...) specifies user callback for all nodes.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'EdgeCallback', *EdgeCallbackValue*, ...) specifies user callback for all edges.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'CustomNodeDrawFcn', *CustomNodeDrawFcnValue*, ...) specifies function handle to customized function to draw nodes. Default is [].

Examples

1 Create a biograph object with default node IDs, and then use the get function to display the node IDs.

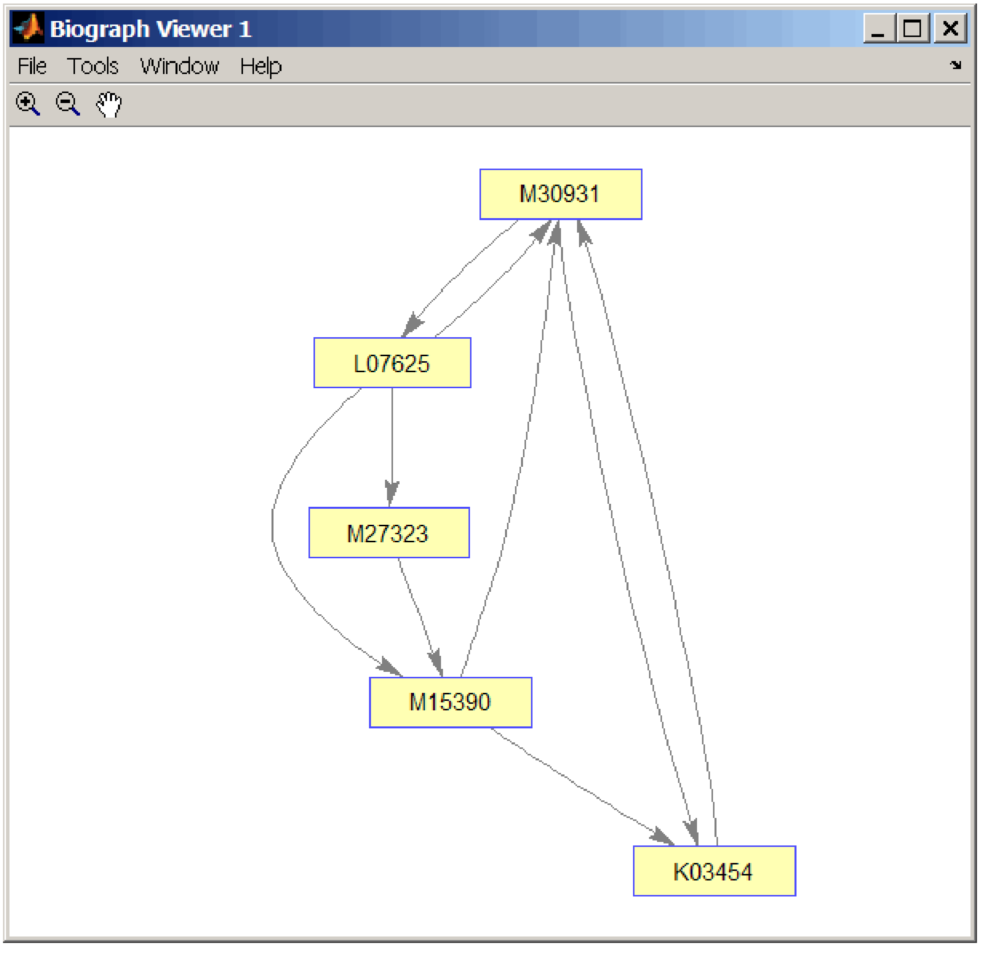
```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
bg1 = biograph(cm)
Biograph object with 5 nodes and 9 edges.
get(bg1.nodes,'ID')

ans =

    'Node 1'
    'Node 2'
    'Node 3'
    'Node 4'
    'Node 5'
```

2 Create a biograph object, assign the node IDs, and then use the get function to display the node IDs.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
ids = {'M30931','L07625','K03454','M27323','M15390'};
bg2 = biograph(cm,ids);
get(bg2.nodes,'ID')

ans =

    'M30931'
    'L07625'
    'K03454'
    'M27323'
    'M15390'
```

3 Use the view method to display the biograph object.

```
view(bg2)
```



See Also

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getmatrix`, `getnodesbyid`, `getrelatives`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`, `traverse`, `view`

MATLAB functions: `get`, `set`

Purpose

Generate remote BLAST request

Syntax

```
blastncbi(Seq, Program)
RID = blastncbi(Seq, Program)
[RID, RTOE] = blastncbi(Seq, Program)
blastncbi(..., 'PropertyName', PropertyValue,...)
blastncbi(..., 'Database', DatabaseValue)
blastncbi(..., 'Descriptions', DescriptionsValue)
blastncbi(..., 'Alignments', AlignmentsValue)
blastncbi(..., 'Filter', FilterValue)
blastncbi(..., 'Expect', ExpectValue)
blastncbi(..., 'Word', WordValue)
blastncbi(..., 'Matrix', MatrixValue)
blastncbi(..., 'GapOpen', GapOpenValue)
blastncbi(..., 'ExtendGap', ExtendGapValue)
blastncbi(..., 'Inclusion', InclusionValue)
blastncbi(..., 'Pct', PctValue)
```

Arguments

Seq	Nucleotide or amino acid sequence. Enter a GenBank or RefSeq accession number, GI, FASTA file, URL, string, character array, or a MATLAB structure that contains the field `Sequence`. You can also enter a structure with the field `Sequence`.
Program	BLAST program. Enter `'blastn'`, `'blastp'`, `'psiblast'`, `'blastx'`, `'tblastn'`, `'tblastx'`, or `'megablast'`.

DatabaseValue	Property to select a database. Compatible databases depend upon the type of sequence submitted and program selected. The nonredundant database, `'nr'`, is the default value for both nucleotide and amino acid sequences. For nucleotide sequences, enter `'nr'`, `'est'`, `'est_human'`, `'est_mouse'`, `'est_others'`, `'gss'`, `'htgs'`, `'pat'`, `'pdb'`, `'month'`, `'alu_repeats'`, `'dbsts'`, `'chromosome'`, `'wgs'`, `'refseq_rna'`, `'refseq_genomic'`, or `'env_nt'`. The default value is `'nr'`. For amino acid sequences, enter `'nr'`, `'swissprot'`, `'pat'`, `'pdb'`,`'month'`, `'refseq_protein'`, or `'env_nr'`, . The default value is `'nr'`.
DescriptionValue	Property to specify the number of short descriptions. The default value is normally `100`, and for `Program = pciblast`, the default value is `500`.
AlignmentValue	Property to specify the number of sequences to report high-scoring segment pairs (HSP). The default value is normally `100`, and for `Program = pciblast`, the default value is `500`.
FilterValue	Property to select a filter. Enter `'L'` (low-complexity), `'R'` (human repeats), `'m'` (mask for lookup table), or `'lcase'` (to turn on the lowercase mask). The default value is `'L'`.
ExpectValue	Property to select the statistical significance threshold. Enter a real number. The default value is `10`.
WordValue	Property to select a word length. For amino acid sequences, `Word` can be `2` or `3` (`3` is the default value), and for nucleotide sequences, Word can be `7`, `11`, or `15` (`11` is the default value). If `Program = 'MegaBlast'`, `Word` can be `11`, `12`, `16`, `20`, `24`, `28`, `32`, `48`, or `64`, with a default value of `28`.

MatrixValue	Property to select a substitution matrix for amino acid sequences. Enter 'PAM30', 'PAM70', 'BLOSUM80', 'BLOSUM62', or 'BLOSUM45'. The default value is 'BLOSUM62'.
InclusionValue	Property for PCI-BLAST searches to define the statistical significance threshold. The default value is 0.005.
PctValue	Property to select the percent identity. Enter None, 99, 98, 95, 90, 85, 80, 75, or 60. Match and mismatch scores are automatically selected. The default value is 99 (99, 1, -3).

Description

The Basic Local Alignment Search Tool (BLAST) offers a fast and powerful comparative analysis of interesting protein and nucleotide sequences against known structures in existing online databases.

`blastncbi(`*`Seq`*`, `*`Program`*`)` sends a BLAST request against a sequence (*Seq*) to NCBI using a specified program (*Program*). With no output arguments, `blastncbi` returns a command window link to the actual NCBI report.

`RID` `= blastncbi(`*`Seq`*`, `*`Program`*`)` calls with one output argument and returns the Report ID (*RID*).

`[`*`RID, RTOE`*`] = blastncbi(`*`Seq`*`, `*`Program`*`)` calls with two output arguments and returns both the report ID (*RID*) and the Request Time Of Execution (*RTOE*) which is an estimate of the time until completion.

`blastncbi` uses the NCBI default values for the optional arguments: `'nr'` for the database, `'L'` for the filter, and `'10'` for the expectation threshold. The default values for the remaining optional arguments depend on which program is used. For help in selecting an appropriate BLAST program, visit

```
http://www.ncbi.nlm.nih.gov/BLAST/producttable.shtml
```

Information for all of the optional parameters can be found at `http://www.ncbi.nlm.nih.gov/staff/tao/URLAPI/blastcgihelp_new.html`

`blastncbi(..., '`*`PropertyName`*`', `*`PropertyValue`*`,...)` defines optional properties using property name/value pairs.

`blastncbi(..., 'Database', `*`DatabaseValue`*`)` selects a database for the alignment search.

`blastncbi(..., 'Descriptions', `*`DescriptionsValue`*`)` , when the function is called without output arguments, specifies the numbers of short descriptions returned to the quantity specified.

`blastncbi(..., 'Alignments', `*`AlignmentsValue`*`)`, when the function is called without output arguments, specifies the number of sequences for which high-scoring segment pairs (HSPs) are reported.

`blastncbi(..., 'Filter', `*`FilterValue`*`)` selects the filter to applied to the query sequence.

`blastncbi(..., 'Expect', `*`ExpectValue`*`)` provides a statistical significance threshold for matches against database sequences. You can learn more about the statistics of local sequence comparison at

`http://www.ncbi.nlm.nih.gov/BLAST/tutorial/Altschul-1.html#head2`

`blastncbi(..., 'Word', `*`WordValue`*`)` selects a word size for amino acid sequences.

`blastncbi(..., 'Matrix', `*`MatrixValue`*`)` selects the substitution matrix for amino acid sequences only. This matrix assigns the score for a possible alignment of two amino acid residues.

`blastncbi(..., 'GapOpen', `*`GapOpenValue`*`)` selects a gap penalty for amino acid sequences. Allowable values for a gap penalty vary with the selected substitution matrix. For information about allowed gap penalties for matrixes other then the `BLOSUM62` matrix, see

`http://www.ncbi.nlm.nih.gov/staff/tao/URLAPI/blastcgihelp_new.html`

`blastncbi(..., 'ExtendGap', `*`ExtendGapValue`*`)` defines the penalty for extending a gap greater than one space.

`blastncbi(..., 'Inclusion', *InclusionValue*)` for PSI-BLAST only, defines the statistical significance threshold (*`InclusionValue`*) for including a sequence in the Position Specific Score Matrix (PSSm) created by PSI-BLAST for the subsequent iteration. The default value is `0.005`.

`blastncbi(..., 'Pct', *PctValue*)`, when *`ProgramValue`* is `'Megablast'`, selects the percent identity and the corresponding match and mismatch score for matching existing sequences in a public database.

Values by Program

	BLASTN	BLASTP	BLASTX	TBLASTN	TBLASTX	MEGA
Database	nr (default), est, est_human, est_mouse, est_others, gss, htgs, pat, pdb, month, alu_repeats, dbsts, chromosome, wgs, refseq_rna, refseq_genomic, env_nt	nr (default), swissprot, pat, pdb, month, refseq_protein, env_nr	values same as BLASTP	values same as BLASTN	values same as BLASTN	values same as BLASTN
Filter	low (default), human, table, lower	low (default), table, lower	low (default), table, lower	low (default), table, lower	low(default), human, table, lower	low
Expect	10(default)	10(default)	10(default)	10 (default)	10 (default)	10
Word	7 11 (default) 15	2 3 (default)	2 3 (default)	2 3 (default)	2 3 (default)	11, 12, 16, 20, 24, 28 (default), 32, 48, 64
Matrix	x	PAM30 PAM70 BLOSUM45 BLOSUM80 BLOSUM62 (default)	PAM30 PAM70 BLOSUM45 BLOSUM80 BLOSUM62 (default)	PAM30 PAM70 BLOSUM45 BLOSUM80 BLOSUM62 (default)	PAM30 PAM70 BLOSUM45 BLOSUM80 BLOSUM62 (default)	x

	BLASTN	BLASTP	BLASTX	TBLASTN	TBLASTX	MEGA
GAP	x	[9 2], [8 2], [7 2], [12 1], [11 1](default), [10 1]	[9 2], [8 2], [7 2], [12 1], [11 1](default), [10 1]	[9 2], [8 2], [7 2], [12 1], [11 1](default), [10 1]	[9 2], [8 2], [7 2], [12 1], [11 1](default), [10 1]	x
Pct	x	x	x	x	x	79, 80, 88. 95, 98, 99 (default)

Examples

```
% Get a sequence from the Protein Data Bank and create
% a MATLAB structure
S = getpdb('1CIV')

% Use the structure as input for a BLAST search with an
% expectation of 1e-10.
blastncbi(S,'blastp','expect',1e-10)

% Click the URL link (Link to NCBI BLAST Request) to go
% directly to the NCBI request.

% You can also try a search directly with an accession
% number and an alternative scoring matrix.
RID = blastncbi('AAA59174','blastp','matrix','PAM70,'...
                             'expect',1e-10)

% The results based on the RID are at
http://www.ncbi.nlm.nih.gov/BLAST/Blast.cgi

% or pass the RID to BLASTREAD to parse the report and
% load it into a MATLAB structure.
blastread(RID)
```

See Also

Bioinformatics Toolbox functions: `blastread`, `getblast`

Purpose

Read data from NCBI BLAST report file

Syntax

```
Data = blastread(File)
```

Arguments

File	NCBI BLAST formatted report file. Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text for a NCBI BLAST report.

Description

BLAST (**B**asic **L**ocal **A**lignment **S**earch **T**ool) reports offer a fast and powerful comparative analysis of interesting protein and nucleotide sequences against known structures in existing online databases. BLAST reports can be lengthy, and parsing the data from the various formats can be cumbersome.

`Data = blastread(File)` reads a BLAST report from an NCBI formatted file (`File`) and returns a data structure (`Data`) containing fields corresponding to the BLAST keywords. `blastread` parses the basic BLAST reports `BLASTN`, `BLASTP`, `BLASTX`, `TBLASTN`, and `TBLASTX`.

`Data` contains the following fields:

Field	Description
`RID`	
`Algorithm`	
`Query`	
`Database`	
`Hits.Name`	
`Hits.Length`	
`Hits.HSP.Score`	
`Hits.HSP.Expect`	

Field	Description
Hits.HSP.Identities	
Hits.HSP.Positives	
Hits.HSP.Gaps	
Hits.HSP.Frame	
Hits.HSP.Strand	
Hits.HSP.Alignment	
Hits.HSPs.QueryIndices	
Hits.HSPs.SubjectIndices	
Statistics	

Examples

1 Create a BLAST request with a GenPept accession number.

```
RID = blastncbi('AAA59174', 'blastp', 'expect', 1e-10)
```

2 Pass the RID to getblast, download the report and save the report to a text file.

```
getblast(RID, 'ToFile' ,'AAA59174_BLAST.rpt')
```

3 Using the saved file, read the results into a MATLAB structure.

```
results = blastread('AAA59174_BLAST.rpt')
```

References

For more information about reading and interpreting BLAST reports, see

http://www.ncbi.nlm.nih.gov/Education/BLASTinfo/Blast_output.html

See Also

Bioinformatics Toolbox functions: blastncbi, getblast

Purpose

BLOSUM scoring matrix

Syntax

```
Matrix = blosum(Identity)
[Matrix, MatrixInfo] = blosum(Identity)
blosum(..., 'PropertyName', PropertyValue,...)
blosum(..., 'Extended', ExtendedValue)
blosum(..., 'Order', OrderValue)
```

Arguments

Identity	Percent identity level. Enter values from 30 to 90 in increments of 5, enter 62, or enter 100.
ExtendedValue	Property to control the listing of extended amino acid codes. Enter either `true` (default) or `false`.
OrderValue	Property to specify the order amino acids are listed in the matrix. Enter a character string of legal amino acid characters. The length is 20 or 24 characters.

Description

`Matrix = blosum(Identity)` returns a BLOSUM (**Blo**cks **Sub**stitution **M**atrix) matrix with a specified percent identity. The default ordering of the output includes the extended characters `B`, `Z`, `X`, and `*`.

```
A R N D C Q E G H I L K M F P S T W Y V B Z X *
```

`[Matrix, MatrixInfo] = blosum(Identity)` returns a structure of information (`MatrixInfo`) about a BLOSUM matrix (`Matrix`) with the fields `Name`, `Scale`, `Entropy`, `ExpectedScore`, `HighestScore`, `LowestScore`, and `Order`.

`blosum(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`blosum(..., 'Extended', ExtendedValue)`, if `Extended` is `false`, returns the scoring matrix for the standard 20 amino acids. Ordering of the output when `Extended` is `false` is

```
A R N D C Q E G H I L K M F P S T W Y V
```

`blosum(..., 'Order', OrderValue)` returns a BLOSUM matrix ordered by an amino acid sequence (*OrderString*).

Examples

Return a BLOSUM matrix with a value of 50.

```
B50 = blosum(50)
```

Return a BLOSUM matrix with the amino acids in a specific order.

```
B75 = blosum(75,'Order','CSTPAGNDEQHRKMILVFYW')
```

See Also

Bioinformatics Toolbox functions `dayhoff`, `gonnet`, `nwalign`, `pam`, `swalign`

Purpose

Read probe intensities from Affymetrix CEL files (Windows 32)

Syntax

```
ProbeStructure = celintensityread(CELFiles, CDFFile)
ProbeStructure = celintensityread(..., 'CELPath',
CELPathValue, ...)
ProbeStructure = celintensityread(..., 'CDFPath',
   CDFPathValue, ...)
ProbeStructure = celintensityread(..., 'PMOnly',
PMOnlyValue,
   ...)
ProbeStructure = celintensityread(..., 'Verbose',
   VerboseValue, ...)
```

Arguments

CELFiles	Cell array of CEL file names. If you set *CELFiles* to `'*'`, then it reads all CEL files in the current directory. If you set *CELFiles* to `' '`, then it opens the Select CEL Files dialog box from which you select the CEL files. From this dialog box, you can press and hold **Ctrl** or **Shift** while clicking to select multiple CEL files.
CDFFile	String specifying a CDF file name. If you set *CDFFile* to `' '`, then it opens the Select CDF File dialog box from which you select the CDF file.
CELPathValue	String specifying the path and directory where the files specified in *CELFiles* are stored.
CDFPathValue	String specifying the path and directory where the file specified in *CDFFile* is stored.

PMOnlyValue	Property to include or exclude the mismatch (MM) probe intensity values in the returned structure. Enter `true` to return only perfect match (PM) probe intensities. Enter `false` to return both PM and MM probe intensities. Default is `true`.
VerboseValue	Controls the display of a progress report showing the name of each CEL file as it is read. When *VerboseValue* is `false`, no progress report is displayed. Default is `true`.

Return Values

ProbeStructure	MATLAB structure containing information from the CEL files, including probe intensities, probe indices, and probe set IDs.

Description

Note This function is supported on the Windows 32 platform only.

ProbeStructure = `celintensityread(`*CELFiles, CDFFile*`)` reads the specified Affymetrix CEL files and the associated CDF library file, and then creates *ProbeStructure*, a structure containing information from the CEL files, including probe intensities, probe indices, and probe set IDs. *CELFiles* is a cell array of CEL file names. *CDFFile* is a string specifying a CDF file name.

If you set *CELFiles* to `'*'`, then it reads all CEL files in the current directory. If you set *CELFiles* to `' '`, then it opens the Select CEL Files dialog box from which you select the CEL files. From this dialog box, you can press and hold **Ctrl** or **Shift** while clicking to select multiple CEL files.

If you set *CDFFile* to `' '`, then it opens the Select CDF File dialog box from which you select the CDF file.

ProbeStructure = `celintensityread(..., '`*PropertyName*`',` *PropertyValue*`, ...)` calls `celintensityread` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

ProbeStructure = celintensityread(..., 'CELPath', *CELPathValue*, ...) specifies a path and directory where the files specified in *CELFiles* are stored.

ProbeStructure = celintensityread(..., 'CDFPath', *CDFPathValue*, ...) specifies a path and directory where the file specified in *CDFFile* is stored.

ProbeStructure = celintensityread(..., 'PMOnly', *PMOnlyValue*, ...) includes or excludes the mismatch (MM) probe intensity values. When *PMOnlyValue* is true, celintensityread returns only perfect match (PM) probe intensities. When *PMOnlyValue* is false, celintensityread returns both PM and MM probe intensities. Default is true.

ProbeStructure contains the following fields.

Field	Description
CDFName	File name of the Affymetrix library CDF file.
CELNames	Cell array of names of the Affymetrix CEL files.
NumProbeSets	Number of probe sets in each CEL file.
ProbeSetIDs	Cell array of the probe set IDs from the Affymetrix CDF library file.
ProbeIndices	Column vector containing probe indexing information. Probes within a probe set are numbered 0 through N - 1, where N is the number of probes in the probe set.

Field	Description
PMIntensities	Matrix containing PM probe intensity values. Each row corresponds to a probe, and each column corresponds to a CEL file. The rows are ordered the same as in ProbeIndices, and the columns are ordered the same as in the *CELFiles* input argument.
MMIntensities	Matrix containing MM probe intensity values. Each row corresponds to a probe, and each column corresponds to a CEL file. The rows are ordered the same as in ProbeIndices, and the columns are ordered the same as in the *CELFiles* input argument.

ProbeStructure = celintensityread(..., 'Verbose', *VerboseValue*, ...) controls the display of a progress report showing the name of each CEL file as it is read. When *VerboseValue* is false, no progress report is displayed. Default is true.

Examples

The following example assumes that you have the HG_U95Av2.CDF library file stored at D:\Affymetrix\LibFiles\HGGenome, and that your Current Directory points to a location containing CEL files associated with this CDF library file. In this example, the celintensityread function reads all the CEL files in the Current Directory and a CDF file in a specified directory. The next command line uses the rmabackadj function to perform background adjustment on the PM probe intensities in the PMIntensities field of PMProbeStructure.

```
PMProbeStructure = celintensityread('*', 'HG_U95Av2.CDF',...
                   'CDFPath', 'D:\Affymetrix\LibFiles\HGGenome');
BackAdjustedMatrix = rmabackadj(PMProbeStructure.PMIntensities);
```

The following example lets you select CEL files and a CDF file to read using Open File dialog boxes:

```
PMProbeStructure = celintensityread(' ', ' ');
```

See Also

Bioinformatics Toolbox functions: `affyread`, `agferead`, `gprread`, `probelibraryinfo`, `probesetlink`, `probesetlookup`, `probesetplot`, `probesetvalues`, `sptread`

classperf

Purpose Evaluate performance of classifier

Syntax

```
classperf
cp = classperf(groundtruth)
classperf(cp, classout)
classperf(cp, classout, testidx)
cp = classperf(groundtruth, classout,...)
cp = classperf(..., 'Positive', PositiveValue, 'Negative',
   NegativeValue)
```

Description

`classperf` provides an interface to keep track of the performance during the validation of classifiers. `classperf` creates and updates a classifier performance object (*`CP`*) that accumulates the results of the classifier. Later, classification standard performance parameters can be accessed using the function `get` or as fields in structures. Some of these performance parameters are ErrorRate, CorrectRate, ErrorDistributionByClass, Sensitivity and Specificity. `classperf`, without input arguments, displays all the available performance parameters.

`cp` `= classperf(`*`groundtruth`*`)` creates and initializes an empty object. *`CP`* is the handle to the object. *`groundtruth`* is a vector containing the true class labels for every observation. *`groundtruth`* can be a numeric vector or a cell array of strings. When used in a cross-validation design experiment, *`groundtruth`* should have the same size as the total number of observations.

`classperf(`*`cp`*`, `*`classout`*`)` updates the *`CP`* object with the classifier output *`classout`*. *`classout`* is the same size and type as *`groundtruth`*. When *`classout`* is numeric and `groundtruth` is a cell array of strings, the function `grp2idx` is used to create the index vector that links `classout` to the class labels. When `classout` is a cell array of strings, an empty string, `''`, represents an inconclusive result of the classifier. For numeric arrays, `NaN` represents an inconclusive result.

`classperf(`*`cp`*`, `*`classout`*`, `*`testidx`*`)` updates the *`CP`* object with the classifier output *`classout`*. *`classout`* has smaller size than *`groundtruth`*, and *`testidx`* is an index vector or a logical index vector of the same size as `groundtruth`, which indicates the observations that were used in the current validation.

`cp = classperf(groundtruth, classout,...)` creates and updates the *CP* object with the first validation. This form is useful when you want to know the performance of a single validation.

`cp = classperf(..., 'Positive', PositiveValue, 'Negative', NegativeValue)` sets the `'positive'` and `'negative'` labels to identify the target disorder and the control classes. These labels are used to compute clinical diagnostic test performance. `p` and `n` must consist of disjoint sets of the labels used in *groundtruth*. For example, if

```
groundtruth = [1 2 2 1 3 4 4 1 3 3 3 2]
```

you could set

```
p = [1 2];
n = [3 4];
```

If *groundtruth* is a cell array of strings, `p` and `n` can either be cell arrays of strings or numeric vectors whose entries are subsets of `grp2idx(groundtruth)`. *PositiveValue* defaults to the first class returned by `grp2idx(groundtruth)`, while *NegativeValue* defaults to all the others. In clinical tests, inconclusive values (`''` or `NaN`) are counted as false negatives for the computation of the specificity and as false positives for the computation of the sensitivity, that is, inconclusive results may decrease the diagnostic value of the test. Tested observations for which true class is not within the union of *PositiveValue* and *NegativeValue* are not considered. However, tested observations that result in a class not covered by the vector `groundtruth` are counted as inconclusive.

Examples

```
% Classify the fisheriris data with a K-Nearest Neighbor
classifier load fisheriris
c = knnclassify(meas,meas,species,4,'euclidean','Consensus');
cp = classperf(species,c)
get(cp)
```

```
% 10-fold cross-validation on the fisheriris data using linear
% discriminant analysis and the third column as only feature for
% classification
load fisheriris
indices = crossvalind('Kfold',species,10);
cp = classperf(species); % initializes the CP object
for i = 1:10
    test = (indices == i); train = ~test;
    class = classify(meas(test,3),meas(train,3),species(train));
    % updates the CP object with the current classification results
    classperf(cp,class,test)
end
cp.CorrectRate % queries for the correct classification rate


cp =

 biolearning.classperformance

                        Label: ''
                  Description: ''
                  ClassLabels: {3x1 cell}
                  GroundTruth: [150x1 double]
         NumberOfObservations: 150
               ControlClasses: [2x1 double]
                TargetClasses: 1
            ValidationCounter: 1
           SampleDistribution: [150x1 double]
            ErrorDistribution: [150x1 double]
    SampleDistributionByClass: [3x1 double]
     ErrorDistributionByClass: [3x1 double]
               CountingMatrix: [4x3 double]
                  CorrectRate: 1
                    ErrorRate: 0
             InconclusiveRate: 0.0733
               ClassifiedRate: 0.9267
                  Sensitivity: 1
```

```
                    Specificity: 0.8900
      PositivePredictiveValue: 0.8197
      NegativePredictiveValue: 1
           PositiveLikelihood: 9.0909
           NegativeLikelihood: 0
                   Prevalence: 0.3333
              DiagnosticTable: [2x2 double]


ans =
    0.9467
```

See Also

Bioinformatics Toolbox functions `knnclassify`, `svmclassify`, `crossvalind`

Statistics Toolbox functions `grp2idx`, `classify`

cleave

Purpose

Cleave amino acid sequence with enzyme

Syntax

```
Fragments = cleave(SeqAA, PeptidePattern, Position)
[Fragments, CuttingSites] = cleave(...)
[Fragments, CuttingSites, Lengths] = cleave(...)
cleave(..., 'PropertyName', PropertyValue,...)
cleave(..., 'PartialDigest', PartialDigestValue)
```

Arguments

SeqAA	Amino acid sequence. Enter a character string or a vector of integers from the table . Examples: `'ARN'` or `[1 2 3]`. You can also enter a structure with the field `Sequence`.
PeptidePattern	Short amino acid sequence to search in a larger sequence. Enter a character string, vector of integers, or a regular expression.
Position	Position on the `PeptidePattern` where the sequence is cleaved. Enter a position within the `PeptidePattern`. Position `0` corresponds to the N terminal end of the `PepetidePattern`.
PartialDigestValue	Property to specify the probability that a cleavage site will be cleaved. Enter a value from `0` to `1` (default).

Description

`Fragments = cleave(SeqAA, PeptidePattern, Position)` cuts an amino acid sequence (*SeqAA*) into parts at the specified cleavage site specified by a peptide pattern and position.

`[Fragments, CuttingSites] = cleave(...)` returns a numeric vector with the indices representing the cleave sites. A `0` (zero) is added to the list, so `numel(Fragments)==numel(CuttingSites)`. You can use *CuttingSites* + 1 to point to the first amino acid of every fragment respective to the original sequence.

[*Fragments, CuttingSites, Lengths*] = cleave(...) returns a numeric vector with the lengths of every fragment.

cleave(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

cleave(..., 'PartialDigest', *PartialDigestValue*) simulates a partial digestion where PartialDigest is the probability of a cleavage site being cut.

The following table lists some common proteases and their cleavage sites.

Protease	Peptide Pattern	Position
Trypsin	[KR](?!P)	1
Chymotrypsin	[WYF](?!P)	1
Glutamine C	[ED](?!P)	1
Lysine C	[K](?!P)	1
Aspartic acid N	D	1

Examples

1 Get a protein sequence from the GenPept database.

```
S = getgenpept('AAA59174')
```

2 Cleave the sequence using trypsin. Trypsin cleaves after K or R when the next residue is not P.

```
[parts, sites, lengths] = cleave(S.Sequence,'[KR](?!P)',1);
    for i=1:10
        fprintf('%5d%5d   %s\n',sites(i),lengths(i),parts{i})
    end

    0    6   MGTGGR
    6    1   R
    7   34   GAAAAPLLVAVAALLLGAAGHLYPGEVCPGMDIR
   41    5   NNLTR
```

```
 46    21    LHELENCSVIEGHLQILLMFK
 67     7    TRPEDFR
 74     6    DLSFPK
 80    12    LIMITDYLLLFR
 92     8    VYGLESLK
100    10    DLFPNLTVIR
```

See Also

Bioinformatics Toolbox functions: `rebasecuts`, `restrict`, `seqshowwords`

MATLAB function: `regexp`

Purpose

Create dendrogram and heat map

Syntax

```
clustergram(Data)
clustergram(Data, ...'RowLabels', RowLabelsValue, ...)
clustergram(Data, ...'ColumnLabels',
ColumnLabelsValue, ...)
clustergram(Data, ...'Pdist', PdistValue, ...)
clustergram(Data, ...'Linkage', LinkageValue, ...)
clustergram(Data, ...'Dendrogram', DendrogramValue, ...)
clustergram(Data, ...'OptimalLeafOrder',
   OptimalLeafOrderValue, ...)
clustergram(Data, ...'ColorMap', ColorMapValue, ...)
clustergram(Data, ...'SymmetricRange', SymmetricRangeValue,
   ...)
clustergram(Data, ...'Dimension', DimensionValue, ...)
clustergram(Data, ...'Ratio', RatioValue, ...)
```

Arguments

Data	Matrix in which each row corresponds to a gene and each column corresponds to a single experiment or microarray.
RowLabelsValue	Vector of numbers or cell array of text strings to label the rows in `Data`.
ColumnLabelsValue	Vector of numbers or cell array of text strings to label the columns in `Data`.

PdistValue	String to specify the distance metric to pass to the `pdist` function (Statistics Toolbox) to use to calculate the pair-wise distances between observations. For information on choices, see the `pdist` function. Default is `euclidean`. **Note** If the distance metric requires extra arguments, then *`PdistValue`* is a cell array. For example, to use the Minkowski distance with exponent `P`, you would use `{'minkowski', P}`.
LinkageValue	String to specify the linkage method to pass to the `linkage` function (Statistics Toolbox) to use to create the hierarchical cluster tree. For information on choices, see the `linkage` function. Default is `average`.
DendrogramValue	Cell array of property name/property value pairs to pass to the `dendrogram` function (Statistics Toolbox) to create the dendrogram plot. For information on choices, see the `dendrogram` function.

OptimalLeafOrderValue	Property to enable or disable the optimal leaf ordering calculation, which determines the leaf order that maximizes the similarity between neighboring leaves. Choices are `true` (enable) or `false` (disable). Default depends on the size of *`Data`*. If the number of rows or columns in *`Data`* is greater than 1000, default is `false`; otherwise, default is `true`. **Note** Disabling the optimal leaf ordering calculation can be useful when working with large data sets because this calculation uses a large amount of memory and can be very time consuming.
ColorMapValue	Either of the following: • M-by-3 matrix of RGB values • Name or function handle of a function that returns a color map Default is `redgreencmap`.
SymmetricRangeValue	Property to force the color range of the heat map to be symmetric around zero. Choices are `true` (default) or `false`.

DimensionValue	Property to specify either a one-dimensional or two-dimensional clustergram. Choices are 1 (default) or 2.
RatioValue	Either of the following: • Scalar • Two-element vector Default is 1/5.

Description

clustergram(*Data*) creates a dendrogram and heat map from the gene expression data in the matrix *Data*. It uses hierarchical clustering with euclidean distance metric and average linkage to generate the hierarchical tree. The clustering is performed on the rows in matrix *Data*, in which the rows correspond to genes and the columns correspond to different microarrays. To cluster the columns instead of the rows, transpose the data using the transpose (') operator.

clustergram(*Data*, ...'*PropertyName*', *PropertyValue*, ...) calls clustergram with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

clustergram(*Data*, ...'RowLabels', *RowLabelsValue*, ...) uses the contents of *RowLabelsValue*, a vector of numbers or cell array of text strings, as labels for the rows in *Data*.

clustergram(*Data*, ...'ColumnLabels', *ColumnLabelsValue*, ...) uses the contents of *ColumnLabelsValue*, a vector of numbers or cell array of text strings, as labels for the columns in *Data*.

clustergram(*Data*, ...'Pdist', *PdistValue*, ...) specifies the distance metric to pass to the pdist function (Statistics Toolbox) to use to calculate the pair-wise distances between observations. *PdistValue* is a string. For information on choices, see the pdist function. Default is euclidean.

Note If the distance metric requires extra arguments, then *PdistValue* is a cell array. For example, to use the Minkowski distance with exponent P, you would use {'minkowski', P}.

---

clustergram(*Data*, ...'Linkage', *LinkageValue*, ...) specifies the linkage method to pass to the linkage function (Statistics Toolbox) to use to create the hierarchical cluster tree. *LinkageValue* is a string. For information on choices, see the linkage function. Default is average.

clustergram(*Data*, ...'Dendrogram', *DendrogramValue*, ...) specifies property name/property value pairs to pass to the dendrogram function (Statistics Toolbox) to create the dendrogram plot. *DendrogramValue* is a cell array of property name/property value pairs. For information on choices, see the dendrogram function.

clustergram(*Data*, ...'OptimalLeafOrder', *OptimalLeafOrderValue*, ...) enables or disables the optimal leaf ordering calculation, which determines the leaf order that maximizes the similarity between neighboring leaves. Choices are true (enable) or false (disable). Default depends on the size of *Data*. If the number of rows or columns in *Data* is greater than 1000, default is false; otherwise, default is true.

Note Disabling the optimal leaf ordering calculation can be useful when working with large data sets because this calculation uses a large amount of memory and can be very time consuming.

---

clustergram(*Data*, ...'ColorMap', *ColorMapValue*, ...) specifies the color map to use to create the clustergram. This controls the colors used to display the heat map. *ColorMapValue* is either a M-by-3 matrix of RGB values or the name or function handle of a function that returns a color map. Default is redgreencmap.

`clustergram(`*`Data`*`, ...'SymmetricRange',` *`SymmetricRangeValue`*`, ...)`, controls whether the color range of the heat map is symmetric around zero. *`SymmetricRangeValue`* can be `true` (default) or `false`.

`clustergram(`*`Data`*`, ...'Dimension',` *`DimensionValue`*`, ...)` specifies whether to create a one-dimensional or two-dimensional clustergram. Choices are `1` (default) or `2`. The one-dimensional clustergram clusters the rows of the data. The two-dimensional clustergram creates the one-dimensional clustergram, and then clusters the columns of the row-clustered data.

`clustergram(`*`Data`*`, ...'Ratio',` *`RatioValue`*`, ...)` specifies the ratio of the space that the dendrogram(s) use in the *X* and *Y* directions, relative to the size of the heat map. If *`RatioValue`* is a scalar, it is used as the ratio for both directions. If *`RatioValue`* is a two-element vector, the first element is used for the *X* ratio, and the second element is used for the *Y* ratio. The *Y* ratio is ignored for one-dimensional clustergrams. Default ratio is `1/5`.

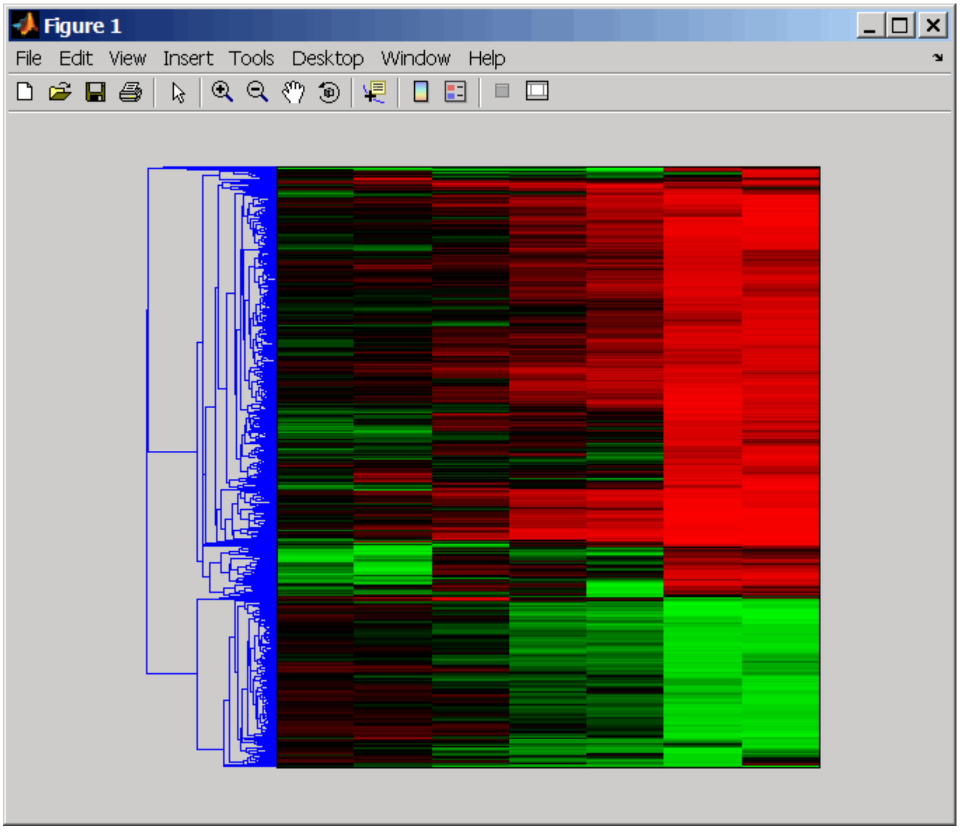
Tip Click and hold the mouse button on the heat map to display the intensity value, column label, and row label for that area of the heat map. View row labels by using the zoom icon to zoom the right side of the clustergram.

Examples

The following example uses data from an experiment (DeRisi et al., 1997) that used DNA microarrays to study temporal gene expression of almost all genes in Saccharomyces cerevisiae during the metabolic shift from fermentation to respiration. Expression levels were measured at seven time points during the diauxic shift.

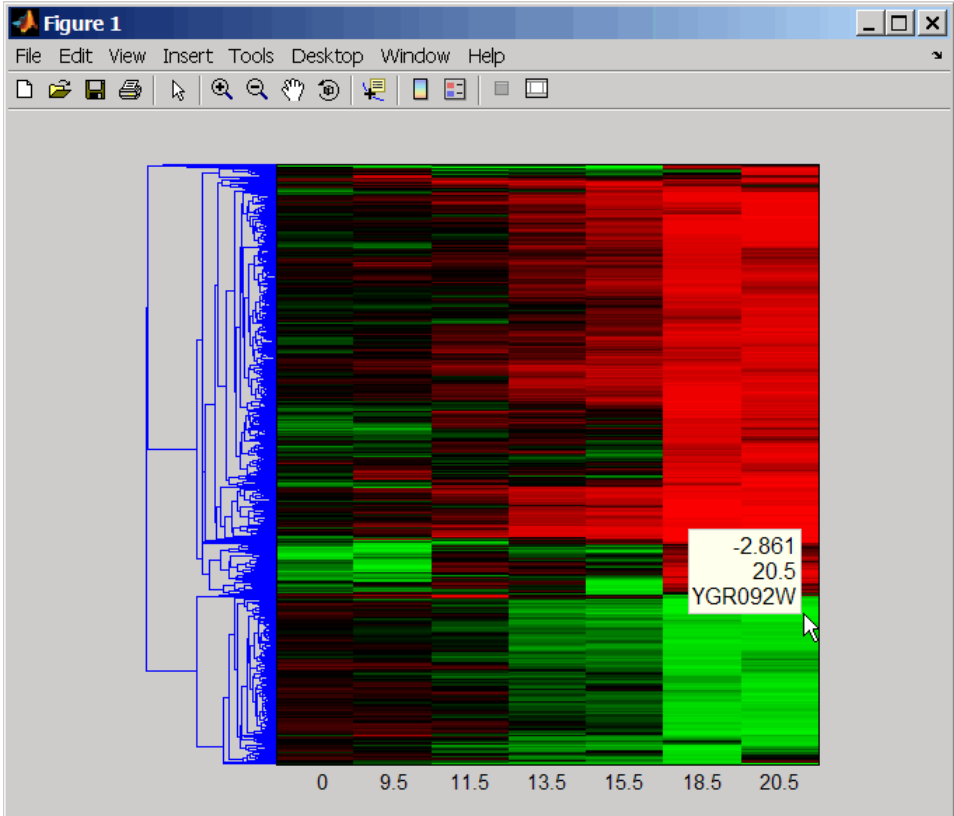
1. Load the filtered yeast data provided with Bioinformatics Toolbox, and then create a clustergram from the gene expression data in the `yeastvalues` matrix.

   ```
   load filteredyeastdata
   clustergram(yeastvalues)
   ```



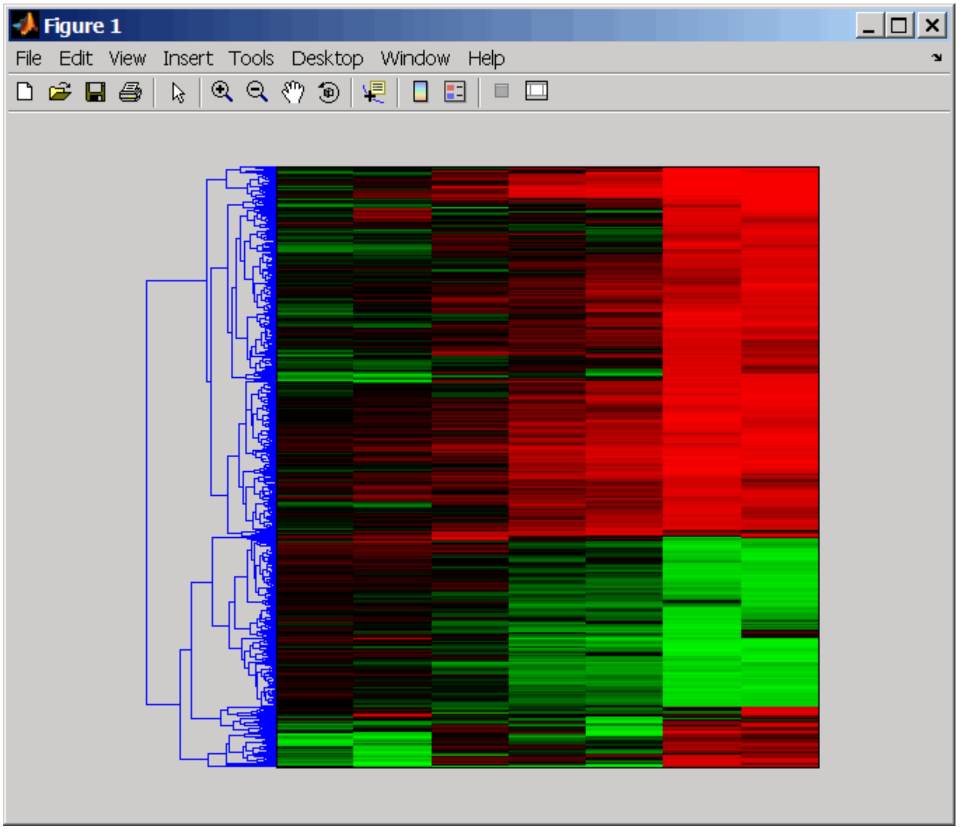
2 Add labels to the clustergram, then click and hold the mouse button on the heat map to display the intensity value, column label, and row label for that area of the heat map. View the row labels by using the Zoom icon to zoom the right side of the clustergram.

```
clustergram(yeastvalues,'RowLabels',genes,'ColumnLabels',times)
```



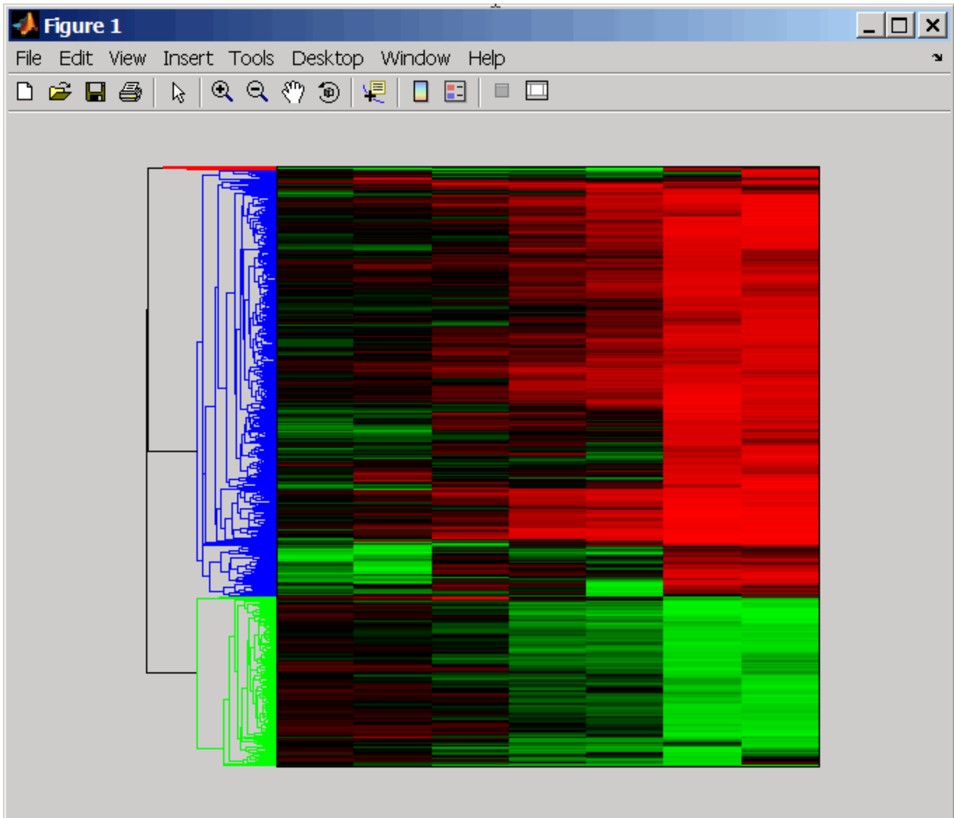
3 Change the clustering parameters.

```
clustergram(yeastvalues,'Linkage','complete')
```



4 Change the color of the groups of nodes in the dendrogram whose linkage is less than a threshold of 5.

```
clustergram(yeastvalues,'RowLabels',genes,...
                        'Dendrogram',{'colorthreshold',5})
```



References

[1] Bar-Joseph, Z., Gifford, D.K., and Jaakkola, T.S. (2001). Fast optimal leaf ordering for hierarchical clustering. Bioinformatics *17*, Suppl 1:S22 – 9. PMID: 11472989.

[2] Eisen, M.B., Spellman, P.T., Brown, P.O., and Botstein, D. (1998). Cluster analysis and display of genome-wide expression patterns. Proc Natl Acad Sci USA *95*, 14863 – 8.

[3] DeRisi, J.L., Iyer, V.R., and Brown, P.O. (1997) Exploring the metabolic and genetic control of gene expression on a genomic scale. Science *278*, 680–686s.

See Also

Bioinformatics Toolbox function: `redgreencmap`

Statistics Toolbox functions: `cluster`, `dendrogram`, `linkage`, `pdist`

codonbias

Purpose

Calculate codon frequency for each amino acid in DNA sequence

Syntax

```
codonbias(SeqDNA)
codonbias(..., 'PropertyName', PropertyValue,...)
codonbias(..., 'GeneticCode', GeneticCodeValue)
codonbias(..., 'Frame', FrameValue)
codonbias(..., 'Reverse', ReverseValue)
codonbias(..., 'Pie', PieValue)
```

Arguments

SeqDNA	Nucleotide sequence (DNA or RNA). Enter a character string with the letters `A`, `T` or `U`, `C`, and `G` or a vector of integers. You can also enter a structure with the field `Sequence`. `codonbias` does not count ambiguous bases or gaps.

Description

Many amino acids are coded by two or more nucleic acid codons. However, the probability that a codon (from the various possible codons for an amino acid) is used to code an amino acid is different between sequences. Knowing the frequency of each codon in a protein coding sequence for each amino acid is a useful statistic.

`codonbias(`*`SeqDNA`*`)` calculates the codon frequency in percent for each amino acid in a DNA sequence (*`SeqDNA`*).

`codonbias(..., '`*`PropertyName`*`',` *`PropertyValue`*`,...)` defines optional properties using property name/value pairs.

`codonbias(..., 'GeneticCode',` *`GeneticCodeValue`*`)` selects an alternative genetic code (*`GenetidCodeValue`*). The default value is `'Standard'` or `1`. For a list of genetic codes, see .

`codonbias(..., 'Frame',` *`FrameValue`*`)` selects a reading frame (*`FrameValue`*). *`FrameValue`* can be `1` (default), `2`, or `3`.

`codonbias(..., 'Reverse',` *`ReverseValue`*`)`, when *`ReverseValue`* is `true`, returns the codon frequency for the reverse complement of the DNA sequence (*`SeqDNA`*).

`codonbias(..., 'Pie', PieValue)`, when *PieValue* is `true`, creates a figure of 20 pie charts for each amino acid.

Example

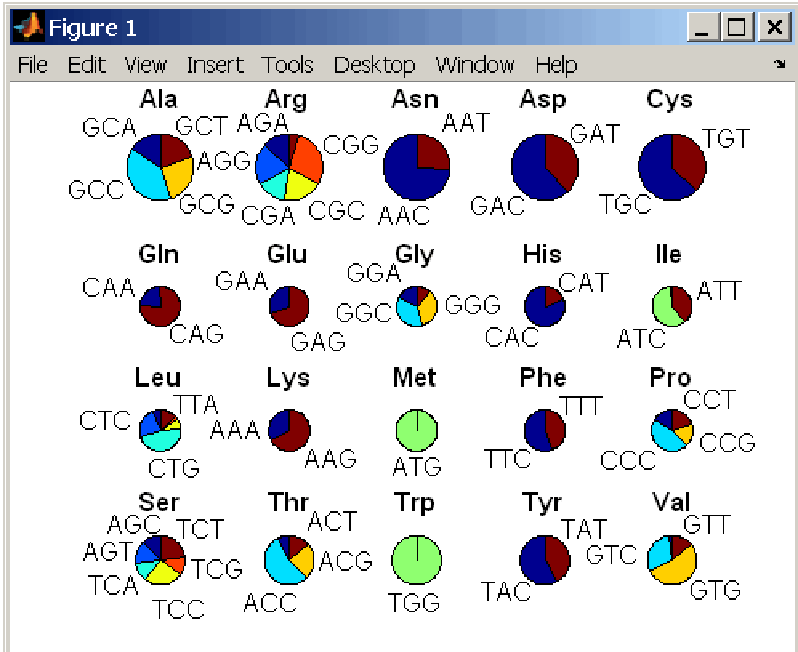
1 Import a nucleotide sequence from GenBank to MATLAB. For example, get the DNA sequence that codes for a human insulin receptor.

```
S = getgenbank('M10051');
```

2 Calculate the codon frequency for each amino acid and plot the results.

```
cb = codonbias(S.Sequence,'PIE',true)

cb.Ala
ans =
    Codon: {'GCA' "GCC' "GCG' 'GCT'}
     Freq: [0.1600 0.3867 0.2533 02000]
```

MATLAB draws a figure with 20 pie charts for the 20 amino acids.



See Also

Bioinformatics Toolbox functions `aminolookup`, `codoncount`, `geneticcode`, `nt2aa`

Purpose

Count codons in nucleotide sequence

Syntax

```
Codons = codoncount(SeqNT)
codoncount(..., 'PropertyName', PropertyValue,...)
codoncount(..., 'Frame', FrameValue)
codoncount(..., 'Reverse', ReverseValue)
codoncount(..., 'Figure', FigureValue)
```

Arguments

SeqNT	Nucleotide sequence. Enter a character string or vector of integers. You can also enter a structure with the field `Sequence`.
FrameValue	Property to select a reading frame. Enter `1` (default), `2`, or `3`.
ReverseValue	Property to control returning the complement sequence. Enter `true` or `false` (default).
FigureValue	Property to control plotting a heat map. Enter either `true` or `false` (default).

Description

`Codons = codoncount(SeqNT)` counts the number of codon in a sequence (*SeqNT*) and returns the codon counts in a structure with the fields `AAA`, `AAC`, `AAG`, ..., `TTG`, `TTT`.

- For sequences that have codons with the character `U`, the `U` characters are added to codons with `T` characters.
- If the sequence contains ambiguous nucleotide characters (`R Y K M S W B D H V N`) , or gaps indicated with a hyphen (`-`), this function creates a field `Others` and displays a warning message.

```
Warning: Ambiguous symbols 'symbol' appear
in the sequence.
These will be in Others.
```

- If the sequence contains undefined nucleotide characters (`E F H I J L O P Q X Z`), `codoncount` ignores the characters and displays a warning message.

```
Warning: Unknown symbols 'symbol' appear
in the sequence.
These will be ignored.
```

[*Codons, CodonArray*] = codoncount(*SeqNT*) returns a 4x4x4 array (*CodonArray*) with the raw count data for each codon. The three dimensions correspond to the three positions in the codon. For example, the element `(2,3,4)` of the array gives the number of `CGT` codons where `A` <=> `1`, `C` <=> `2`, `G` <=> `3`, and `T` <=> `4`.

`codoncount(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`codoncount(..., 'Frame', FrameValue)` counts the codons in a specific reading frame.

`codoncount(..., 'Reverse', ReverseValue)`, when *ReverseValue* is `true`, counts the codons for the reverse complement of the sequence.

`codoncount(..., 'Figure', FigureValue)`, when *FigureValue* is `true` displays a figure showing a heat map of the codon counts.

Examples

Count the number of standard codons in a nucleotide sequence.

```
codons = codoncount('AAACGTTA')

codons =
       AAA: 1  ATC: 0  CGG: 0  GCT: 0  TCA: 0
       AAC: 0  ATG: 0  CGT: 1  GGA: 0  TCC: 0
       AAG: 0  ATT: 0  CTA: 0  GGC: 0  TCG: 0
       AAT: 0  CAA: 0  CTC: 0  GGG: 0  TCT: 0
       ACA: 0  CAC: 0  CTG: 0  GGT: 0  TGA: 0
       ACC: 0  CAG: 0  CTT: 0  GTA: 0  TGC: 0
       ACG: 0  CAT: 0  GAA: 0  GTC: 0  TGG: 0
       ACT: 0  CCA: 0  GAC: 0  GTG: 0  TGT: 0
```

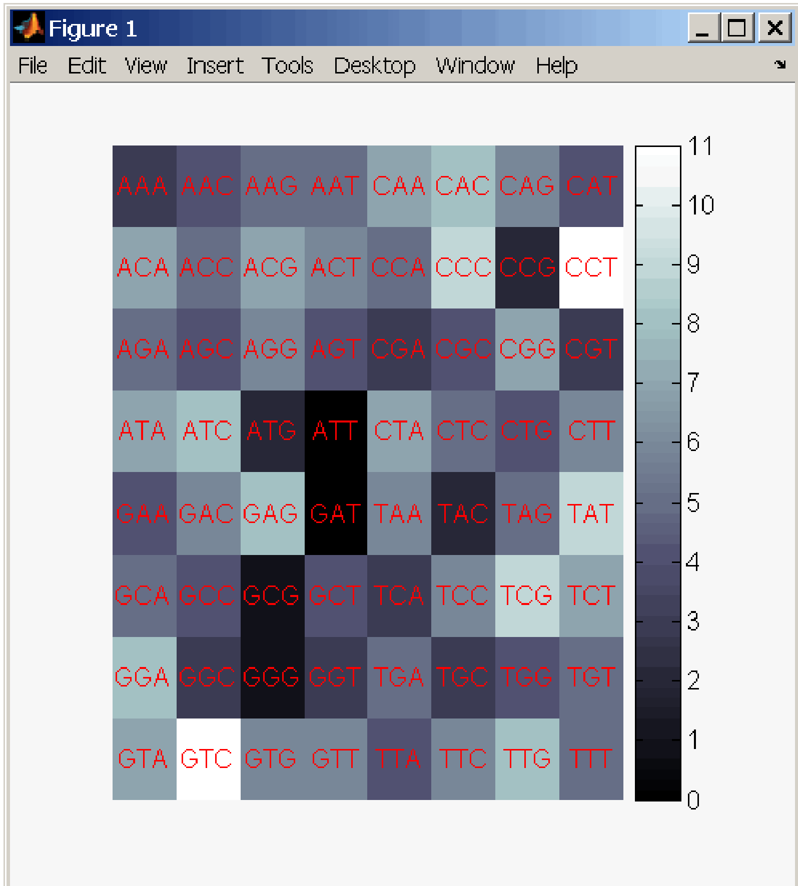
```
AGA: 0  CCC: 0  GAG: 0  GTT: 0  TTA: 0
AGC: 0  CCG: 0  GAT: 0  TAA: 0  TTC: 0
AGG: 0  CCT: 0  GCA: 0  TAC: 0  TTG: 0
AGT: 0  CGA: 0  GCC: 0  TAG: 0  TTT: 0
ATA: 0  CGC: 0  GCG: 0  TAT: 0
```

Count the codons in the second frame for the reverse complement of a sequence.

```
r2codons = codoncount('AAACGTTA', 'Frame',2,...
                                  'Reverse',true);
```

Create a heat map for the codons in a nucleotide sequence.

```
a = randseq(1000);
codoncount(a,'Figure', true);
```



See Also

Bioinformatics Toolbox functions `aacount` , `basecount`, `baselookup`, `codonbias`, `dimercount`, `nmercount`, `ntdensity`, `seqrcomplement`, `seqwordcount`

Purpose

Locate CpG islands in DNA sequence

Syntax

```
cpgisland(SeqDNA)
cpgisland(..., 'PropertyName', PropertyValue,...)
cpgisland(..., 'Window', WindowValue)
cpgisland(..., 'MinIsland', MinIslandValue)
cpgisland(..., 'CpGoe', CpGoeValue)
cpgisland(..., 'GCmin', GCminValue)
cpgisland(..., 'Plot', PlotValue)
```

Arguments

SeqDNA	DNA nucleotide sequence. Enter a character string with the letters `A`, `T`, `C`, and `G`. You can also enter a structure with the field `Sequence`. `cpgisland` does not count ambiguous bases or gaps.

Description

`cpgisland(`*`SeqDNA`*`)` finds CpG islands by marking bases within a moving window of `100` DNA bases with a `GC` content greater than 50% and a `CpGobserved/CpGexpected` ratio greater than 60%.

`cpgisland(..., '`*`PropertyName`*`',` *`PropertyValue`*`,...)` defines optional properties using property name/value pairs.

`cpgisland(..., 'Window',` *`WindowValue`*`)` specifies the window size for calculating GC percent and `CpGobserved/CpGexpected` ratios for a sequence. The default value is `100` bases. A smaller window size increases the noise in a plot.

`cpgisland(..., 'MinIsland',` *`MinIslandValue`*`)` specifies the minimum number of consecutive marked bases to report. The default value is `200` bases.

`cpgisland(..., 'CpGoe',` *`CpGoeValue`*`)` specifies the minimum `CpGobserved/CpGexpected` ratio in each window needed to mark a base. Enter a value between 0 and 1. The default value is `0.6`. This ratio is defined as

```
CPGobs/CpGexp = (NumCpGs*Length)/(NumGs*NumCs)
```

`cpgisland(..., 'GCmin', GCminValue)` specifies the minimum GC percent in a window needed to mark a base. Enter a value between 0 and 1. The default value is `0.5`.

`cpgisland(..., 'Plot', PlotValue)`, when `Plot` is `true`, plots GC content, CpGoe content, CpG islands greater than the minimum island size, and all potential CpG islands for the specified criteria.

Example

1. Import a nucleotide sequence from GenBank. For example, get a sequence from Homo Sapiens chromosome 12.

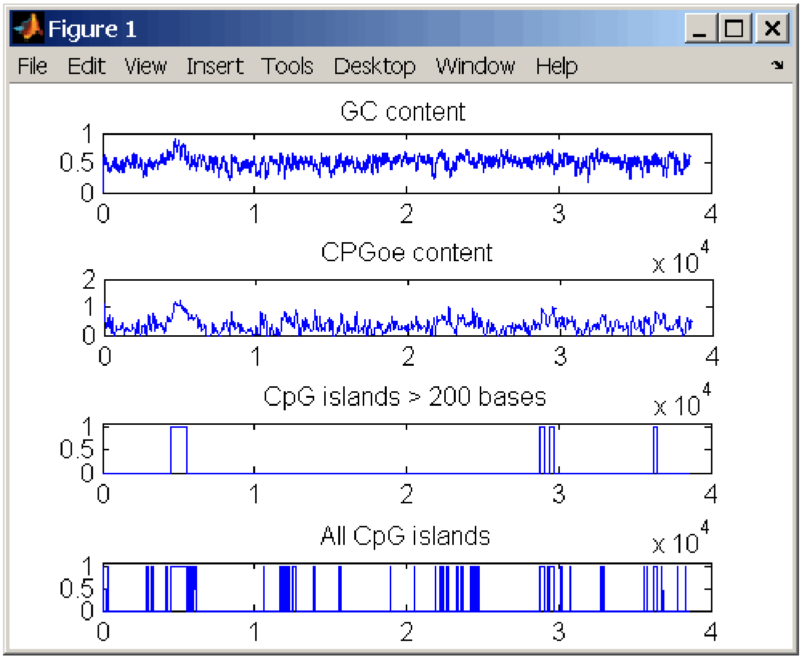
   ```
   S = getgenbank('AC156455');
   ```

2. Calculate the CpG islands in the sequence and plot the results.

   ```
   cpgisland(S.Sequence,'PLOT',true)
   ```

   MATLAB lists the CpG islands greater than 200 bases and draws a figure.

   ```
   ans =
      Starts: [4470 28753 29347 36229]
      Stops: [5555 29064 29676 36450]
   ```



See Also

Bioinformatics Toolbox functions: `basecount`, `ntdensity`, `seqshoworfs`

Purpose

Generate cross-validation indices

Syntax

```
Indices = crossvalind('Kfold', N, K)
[Train, Test] = crossvalind('HoldOut', N, P)
[Train, Test] = crossvalind('LeaveMOut', N, M)
[Train, Test] = crossvalind('Resubstitution', N, [P,Q])
[...] = crossvalind(Method, Group, ...)
[...] = crossvalind(Method, Group, ..., 'Classes', C)
[...] = crossvalind(Method, Group, ..., 'Min', MinValue)
```

Description

`Indices = crossvalind('Kfold', N, K)` returns randomly generated indices for a K-fold cross-validation of `N` observations. `Indices` contains equal (or approximately equal) proportions of the integers `1` through `K` that define a partition of the `N` observations into `K` disjoint subsets. Repeated calls return different randomly generated partitions. `K` defaults to `5` when omitted. In K-fold cross-validation, `K-1` folds are used for training and the last fold is used for evaluation. This process is repeated `K` times, leaving one different fold for evaluation each time.

`[Train, Test] = crossvalind('HoldOut', N, P)` returns logical index vectors for cross-validation of `N` observations by randomly selecting `P*N` (approximately) observations to hold out for the evaluation set. `P` must be a scalar between `0` and `1`. P defaults to `0.5` when omitted, corresponding to holding `50%` out. Using holdout cross-validation within a loop is similar to K-fold cross-validation one time outside the loop, except that non-disjointed subsets are assigned to each evaluation.

`[Train, Test] = crossvalind('LeaveMOut', N, M)`, where `M` is an integer, returns logical index vectors for cross-validation of `N` observations by randomly selecting `M` of the observations to hold out for the evaluation set. `M` defaults to `1` when omitted. Using `LeaveMOut` cross-validation within a loop does not guarantee disjointed evaluation sets. Use K-fold instead.

`[Train, Test] = crossvalind('Resubstitution', N, [P,Q])` returns logical index vectors of indices for cross-validation of `N` observations by randomly selecting `P*N` observations for the evaluation set and `Q*N` observations for training. Sets are selected in order to minimize the number of observations that are used in both sets. P and Q are scalars between 0 and 1. Q=1-P corresponds to holding out (100*P)%, while P=Q=1 corresponds to full resubstitution. [P,Q] defaults to [1,1] when omitted.

[...] = crossvalind(Method, Group, ...) takes the group structure of the data into account. Group is a grouping vector that defines the class for each observation. Group can be a numeric vector, a string array, or a cell array of strings. The partition of the groups depends on the type of cross-validation: For K-fold, each group is divided into K subsets, approximately equal in size. For all others, approximately equal numbers of observations from each group are selected for the evaluation set. In both cases the training set contains at least one observation from each group.

[...] = crossvalind(Method, Group, ..., 'Classes', C) restricts the observations to only those values specified in C. C can be a numeric vector, a string array, or a cell array of strings, but it is of the same form as Group. If one output argument is specified, it contains the value 0 for observations belonging to excluded classes. If two output arguments are specified, both will contain the logical value false for observations belonging to excluded classes.

[...] = crossvalind(Method, Group, ..., 'Min', MinValue) sets the minimum number of observations that each group has in the training set. Min defaults to 1. Setting a large value for Min can help to balance the training groups, but adds partial resubstitution when there are not enough observations. You cannot set Min when using K-fold cross-validation.

Examples

Create a 10-fold cross-validation to compute classification error.

```
load fisheriris
indices = crossvalind('Kfold',species,10);
cp = classperf(species);
for i = 1:10
    test = (indices == i); train = ~test;
    class = classify(meas(test,:),meas(train,:),species(train,:));
```

```
    classperf(cp,class,test)
end
cp.ErrorRate
```

Approximate a leave-one-out prediction error estimate.

```
load carbig
x = Displacement; y = Acceleration;
N = length(x);
sse = 0;
for i = 1:100
    [train,test] = crossvalind('LeaveMOut',N,1);
    yhat = polyval(polyfit(x(train),y(train),2),x(test));
    sse = sse + sum((yhat - y(test)).^2);
end
CVerr = sse / 100
```

Divide cancer data 60/40 without using the `'Benign'` observations. Assume groups are the true labels of the observations.

```
labels = {'Cancer','Benign','Control'};
groups = labels(ceil(rand(100,1)*3));
[train,test] = crossvalind('holdout',groups,0.6,'classes',...
                           {'Control','Cancer'});
sum(test) % Total groups allocated for testing
sum(train) % Total groups allocated for training
```

See Also

Bioinformatics Toolbox functions: `classperf`, `knnclassify`, `svmclassify`

Statistics Toolbox functions: `classify`, `grp2idx`

Purpose

Dayhoff scoring matrix

Syntax

`ScoringMatrix = dayhoff`

Description

ScoringMatrix = dayhoff returns a PAM250 type scoring matrix. The order of amino acids in the matrix is A R N D C Q E G H I L K M F P S T W Y V B Z X *.

See Also

Bioinformatics Toolbox functions: blosum, gonnet, pam

dimercount

Purpose

Count dimers in sequence

Syntax

```
Dimers = dimercount(SeqNT)
[Dimers, Percent] = dimercount(SeqNT)
dimercount(..., 'PropertyName', PropertyValue,...)
dimercount(..., 'Chart', ChartStyle)
```

Arguments

SeqNT	Nucleotide sequence. Enter a character string or vector of integers. Examples: `'ACGT'` and `[1 2 3 4]`.You can also enter a structure with the field `Sequence`.
ChartStyleValue	Property to select the type of plot. Enter `'pie'` or `'bar'`.

Description

`Dimers = dimercount(SeqNT)` counts the number of nucleotide dimers in a 1-by-1 sequence and returns the dimer counts in a structure with the fields `AA`, `AC`, `AG`, `AT`, `CA`, `CC`, `CG`, `CT`, `GA`, `GC`, `GG`, `GT`, `TA`, `TC`, `TG`, `TT`.

- For sequences that have dimers with the character `U`, the `U` characters are added to dimers with `T` characters.
- If the sequence contains ambiguous nucleotide characters (`R Y K M S W B D H V N`) , or gaps indicated with a hyphen (`-`), this function creates a field `Others` and displays a warning message.

  ```
  Warning: Ambiguous symbols 'symbol list' appear
  in the sequence.
  These will be in Others.
  ```

- If the sequence contains undefined nucleotide characters (`E F H I J L O P Q X Z`), `codoncount` ignores the characters and displays a warning message.

```
Warning: Unknown symbols 'symbol list' appear
in the sequence.
These will be ignored.
```

[*Dimers, Percent*] = dimercount(*SeqNT*) returns a 4-by-4 matrix with the relative proportions of the dimers in SeqNT. The rows correspond to A, C, G, and T in the first element of the dimer, and the columns correspond to A, C, G, and T in the second element.

dimercount(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

dimercount(..., 'Chart', *ChartStyle*) creates a chart showing the relative proportions of the dimers.

Examples

Count the number of dimers in a nucleotide sequence.

```
dimercount('TAGCTGGCCAAGCGAGCTTG')

ans =
    AA: 1
    AC: 0
    AG: 3
    AT: 0
    CA: 1
    CC: 1
    CG: 1
    CT: 2
    GA: 1
    GC: 4
    GG: 1
    GT: 0
    TA: 1
    TC: 0
    TG: 2
    TT: 1
```

See Also

Bioinformatics Toolbox functions `aacount`, `basecount`, `baselookup`, `codoncount`, `nmercount`, `ntdensity`

Purpose

Convert DNA sequence to RNA sequence

Syntax

`SeqRNA = dna2rna(SeqDNA)`

Arguments

SeqDNA	DNA sequence. Enter either a character string with the characters `A`, `T`, `G`, `C`, and ambiguous characters `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, `V`, `N`, or a vector of integers from the table Mapping Nucleotide Letters to Integers on page 2-518. You can also enter a structure with the field `Sequence`.
SeqRNA	RNA sequence.

Description

`SeqRNA = dna2rna(SeqDNA)` converts a DNA sequence to an RNA sequence by converting any thymine nucleotides (`T`) in the DNA sequence to uracil (`U`). The RNA sequence is returned in the same format as the DNA sequence. For example, if *SeqDNA* is a vector of integers, then so is *SeqRNA*.

Examples

Convert a DNA sequence to an RNA sequence.

```
rna = dna2rna('ACGATGAGTCATGCTT')

rna =
ACGAUGAGUCAUGCUU
```

See Also

Bioinformatics Toolbox function: `rna2dna`

MATLAB functions: `regexp`, `strrep`

Purpose Estimate synonymous and nonsynonymous substitution rates

Syntax

```
[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2)
[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2,
...'GeneticCode', GeneticCodeValue, ...)
[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2, ...'Method',
   MethodValue, ...)
[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2, ...'Window',
   WindowValue, ...)
[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2, ...'Verbose',
   VerboseValue, ...)
```

Arguments

SeqNT1, *SeqNT2*	Nucleotide sequences. Enter either a string or a structure with the field `Sequence`.
GeneticCodeValue	Property to specify a genetic code. Enter a Code Number or a string with a Code Name from the table . If you use a Code Name, you can truncate it to the first two characters. Default is `1` or `Standard`.

MethodValue	String specifying the method for calculating substitution rates. Choices are: • `NG` (default) — Nei-Gojobori method (1986) uses the number of synonymous and nonsynonymous substitutions and the number of potentially synonymous and nonsynonymous sites. Based on the Jukes-Cantor model. • `LWL` — Li-Wu-Luo method (1985) uses the number of transitional and transversional substitutions at three different levels of degeneracy of the genetic code. Based on Kimura's two-parameter model. • `PBL` — Pamilo-Bianchi-Li method (1993) is similar to the Li-Wu-Luo method, but with bias correction. Use this method when the number of transitions is much larger than the number of transversions.
WindowValue	Integer specifying the sliding window size, in codons, for calculating substitution rates and variances.
VerboseValue	Property to control the display of the codons considered in the computations and their amino acid translations. Choices are `true` or `false` (default). **Tip** Specify `true` to use this display to manually verify the codon alignment of the two input sequences. The presence of stop codons (`*`) in the amino acid translation can indicate that *SeqNT1* and *SeqNT2* are not codon-aligned.

Return Values

Dn	Nonsynonymous substitution rate(s).
Ds	Synonymous substitution rate(s).
Vardn	Variance for the nonsynonymous substitution rate(s).
Vards	Variance for the synonymous substitutions rate(s).

Description

`[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2)` estimates the synonymous and nonsynonymous substitution rates per site between the two homologous nucleotide sequences, *SeqNT1* and *SeqNT2*, by comparing codons using the Nei-Gojobori method.

`dnds` returns:

- *Dn* — Nonsynonymous substitution rate(s).
- *Ds* — Synonymous substitution rate(s).
- *Vardn* — Variance for the nonsynonymous substitution rate(s).
- *Vards* — Variance for the synonymous substitutions rate(s)

This analysis:

- Assumes that the nucleotide sequences, *SeqNT1* and *SeqNT2*, are codon-aligned, that is, do not have frame shifts.

Tip If your sequences are not codon-aligned, use the `nt2aa` function to convert them to amino acid sequences, use the `nwalign` function to globally align them, then use the `seqinsertgaps` function to recover the corresponding codon-aligned nucleotide sequences. See Estimating Synonymous and Nonsynonymous Substitution Rates Between Two Nucleotide Sequences That Are Not Codon-Aligned on page 2-123.

- Excludes codons that include ambiguous nucleotide characters or gaps
- Considers the number of codons in the shorter of the two nucleotide sequences

---

Caution

If *SeqNT1* and *SeqNT2* are too short or too divergent, saturation can be reached, and dnds returns NaNs and a warning message.

[*Dn, Ds, Vardn, Vards*] = dnds(*SeqNT1*, *SeqNT2*, ...'*PropertyName*', *PropertyValue*, ...) calls dnds with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

[*Dn, Ds, Vardn, Vards*] = dnds(*SeqNT1*, *SeqNT2*, ...'GeneticCode', *GeneticCodeValue*, ...) calculates synonymous and nonsynonymous substitution rates using the specified genetic code. Enter a Code Number or a string with a Code Name from the table. If you use a Code Name, you can truncate it to the first two characters. Default is 1 or Standard.

[*Dn, Ds, Vardn, Vards*] = dnds(*SeqNT1*, *SeqNT2*, ...'Method', *MethodValue*, ...) allows you to calculate synonymous and nonsynonymous substitution rates using the following algorithms:

- NG (default) — Nei-Gojobori method (1986) uses the number of synonymous and nonsynonymous substitutions and the number of potentially synonymous and nonsynonymous sites. Based on the Jukes-Cantor model.
- LWL — Li-Wu-Luo method (1985) uses the number of transitional and transversional substitutions at three different levels of degeneracy of the genetic code. Based on Kimura's two-parameter model.

- `PBL` — Pamilo-Bianchi-Li method (1993) is similar to the Li-Wu-Luo method, but with bias correction. Use this method when the number of transitions is much larger than the number of transversions.

`[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2, ...'Window', WindowValue, ...)` performs the calculations over a sliding window, specified in codons. Each output is an array containing a rate or variance for each window.

`[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2, ...'Verbose', VerboseValue, ...)` controls the display of the codons considered in the computations and their amino acid translations. Choices are `true` or `false` (default).

Tip Specify `true` to use this display to manually verify the codon alignment of the two input sequences, *SeqNT1* and *SeqNT2*. The presence of stop codons (`*`) in the amino acid translation can indicate that *SeqNT1* and *SeqNT2* are not codon-aligned.

Examples

Estimating Synonymous and Nonsynonymous Substitution Rates Between the gag Genes of Two HIV Viruses

1. Retrieve two sequences from the GenBank database for the gag genes of two HIV viruses.

```
gag1 = getgenbank('L11768');
gag2 = getgenbank('L11770');
```

2. Estimate the synonymous and nonsynonymous substitution rates between the two sequences.

```
[dn ds vardn vards] = dnds(gag1, gag2)

dn =

    0.0241
```

```
ds =

    0.0739

vardn =

  2.2785e-005

vards =

  2.6447e-004
```

Estimating Synonymous and Nonsynonymous Substitution Rates Between Two Nucleotide Sequences That Are Not Codon-Aligned

1 Retrieve two nucleotide sequences from the GenBank database for the neuraminidase (NA) protein of two strains of the Influenza A virus (H5N1).

```
hk01 = getgenbank('AF509094');
vt04 = getgenbank('DQ094287');
```

2 Extract the coding region from the two nucleotide sequences.

```
hk01_cds = featuresparse(hk01,'feature','CDS','Sequence',true);
vt04_cds = featuresparse(vt04,'feature','CDS','Sequence',true);
```

3 Align the amino acids sequences converted from the nucleotide sequences.

```
[sc,al] = nwalign(nt2aa(hk01_cds),nt2aa(vt04_cds),'extendgap',1);
```

4 Use the `seqinsertgaps` function to copy the gaps from the aligned amino acid sequences to their corresponding nucleotide sequences, thus codon-aligning them.

```
hk01_aligned = seqinsertgaps(hk01_cds,al(1,:))
vt04_aligned = seqinsertgaps(vt04_cds,al(3,:))
```

5 Estimate the synonymous and nonsynonymous substitutions rates of the codon-aligned nucleotide sequences and also display the codons considered in the computations and their amino acid translations.

```
[dn,ds] = dnds(hk01_aligned,vt04_aligned,'verbose',true)
```

References

[1] Li, W., Wu, C., and Luo, C. (1985). A new method for estimating synonymous and nonsynonymous rates of nucleotide substitution considering the relative likelihood of nucleotide and codon changes. Molecular Biology and Evolution *2(2)*, 150–174.

[2] Nei, M., and Gojobori, T. (1986). Simple methods for estimating the numbers of synonymous and nonsynonymous nucleotide substitutions. Molecular Biology and Evolution *3(5)*, 418–426.

[3] Nei, M., and Jin, L. (1989). Variances of the average numbers of nucleotide substitutions within and between populations. Molecular Biology and Evolution *6(3)*, 290–300.

[4] Nei, M., and Kumar, S. (2000). Synonymous and nonsynonymous nucleotide substitutions" in Molecular Evolution and Phylogenetics (Oxford University Press).

[5] Pamilo, P., and Bianchi, N. (1993). Evolution of the Zfx And Zfy genes: rates and interdependence between the genes. Molecular Biology and Evolution *10(2)*, 271–281.

See Also

Bioinformatics Toolbox functions: `dndsml`, `featuresparse`, `geneticcode`, `nt2aa`, `nwalign`, `seqinsertgaps`, `seqpdist`

Purpose

Estimate synonymous and nonsynonymous substitution rates using maximum likelihood method

Syntax

```
[Dn, Ds, Like] = dndsml(SeqNT1, SeqNT2)
[Dn, Ds, Like] = dndsml(SeqNT1, SeqNT2, ...'GeneticCode',
GeneticCodeValue, ...)
[Dn, Ds, Like] = dndsml(SeqNT1, SeqNT2, ...'Verbose',
   VerboseValue, ...)
```

Arguments

SeqNT1, *SeqNT2*	Nucleotide sequences. Enter either a string or a structure with the field `Sequence`.
GeneticCodeValue	Property to specify a genetic code. Enter a Code Number or a string with a Code Name from the table . If you use a Code Name, you can truncate it to the first two characters. Default is `1` or `Standard`.
VerboseValue	Property to control the display of the codons considered in the computations and their amino acid translations. Choices are `true` or `false` (default).

Tip Specify `true` to use this display to manually verify the codon alignment of the two input sequences. The presence of stop codons (`*`) in the amino acid translation can indicate that *SeqNT1* and *SeqNT2* are not codon-aligned.

Return Values

Dn	Nonsynonymous substitution rate(s).
Ds	Synonymous substitution rate(s).
Like	Likelihood of estimate of substitution rates.

Description

[*Dn*, *Ds*, *Like*] = dndsml(*SeqNT1*, *SeqNT2*) estimates the synonymous and nonsynonymous substitution rates between the two homologous sequences, *SeqNT1* and *SeqNT2*, using the Yang-Nielsen method (2000). This maximum likelihood method estimates an explicit model for codon substitution that accounts for transition/transversion rate bias and base/codon frequency bias. Then it uses the model to correct synonymous and nonsynonymous counts to account for multiple substitutions at the same site. The maximum likelihood method is best suited when the sample size is significant (larger than 100 bases) and when the sequences being compared can have transition/transversion rate biases and base/codon frequency biases.

`dndsml` returns:

- *Dn* — Nonsynonymous substitution rate(s).
- *Ds* — Synonymous substitution rate(s).
- *Like* — Likelihood of this estimate.

This analysis:

- Assumes that the nucleotide sequences, *SeqNT1* and *SeqNT2*, are codon-aligned, that is, do not have frame shifts.

> **Tip** If your sequences are not codon-aligned, use the `nt2aa` function to convert them to amino acid sequences, use the `nwalign` function to globally align them, then use the `seqinsertgaps` function to recover the corresponding codon-aligned nucleotide sequences. See Estimating Synonymous and Nonsynonymous Substitution Rates Between Two Nucleotide Sequences That Are Not Codon-Aligned on page 2-128

- Excludes any ambiguous nucleotide characters or codons that include gaps.

- Considers the number of codons in the shorter of the two nucleotide sequences.

Caution

If *SeqNT1* and *SeqNT2* are too short or too divergent, saturation can be reached, and `dndsml` returns `NaN`s and a warning message.

`[`*`Dn, Ds, Like`*`] = dndsml(`*`SeqNT1`*`, `*`SeqNT2`*`, ...'`*`PropertyName`*`',` *`PropertyValue`*`, ...)` calls `dnds` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`[`*`Dn, Ds, Like`*`] = dndsml(`*`SeqNT1`*`, `*`SeqNT2`*`, ...'GeneticCode',` *`GeneticCodeValue`*`, ...)` calculates synonymous and nonsynonymous substitution rates using the specified genetic code. Enter a Code Number or a string with a Code Name from the table. If you use a Code Name, you can truncate it to the first two characters. Default is `1` or `Standard`.

`[`*`Dn, Ds, Like`*`] = dndsml(`*`SeqNT1`*`, `*`SeqNT2`*`, ...'Verbose',` *`VerboseValue`*`, ...)` controls the display of the codons considered in the computations and their amino acid translations. Choices are `true` or `false` (default).

Tip Specify `true` to use this display to manually verify the codon alignment of the two input sequences, *SeqNT1* and *SeqNT2*. The presence of stop codons (`*`) in the amino acid translation can indicate that *SeqNT1* and *SeqNT2* are not codon-aligned.

Examples

Estimating Synonymous and Nonsynonymous Substitution Rates Between the gag Genes of Two HIV Viruses

1 Retrieve two sequences from the GenBank database for the gag genes of two HIV viruses

```
gag1 = getgenbank('L11768');
gag2 = getgenbank('L11770');
```

2 Estimate the synonymous and nonsynonymous substitution rates between the two sequences.

```
[dn ds like] = dndsml(gag1, gag2)

dn =
    0.0259
ds =
    0.0624
like =
   -2.1864e+003
```

Estimating Synonymous and Nonsynonymous Substitution Rates Between Two Nucleotide Sequences That Are Not Codon-Aligned

1 Retrieve two nucleotide sequences from the GenBank database for the neuraminidase (NA) protein of two strains of the Influenza A virus (H5N1).

```
 hk01 = getgenbank('AF509094');
 vt04 = getgenbank('DQ094287');
```

2 Extract the coding region from the two nucleotide sequences.

```
hk01_cds = featuresparse(hk01,'feature','CDS','Sequence',true);
vt04_cds = featuresparse(vt04,'feature','CDS','Sequence',true);
```

3 Align the amino acids sequences converted from the nucleotide sequences.

```
[sc,al]=nwalign(nt2aa(hk01_cds),nt2aa(vt04_cds),'extendgap',1);
```

4 Use the seqinsertgaps function to copy the gaps from the aligned amino acid sequences to their corresponding nucleotide sequences, thus codon-aligning them.

```
hk01_aligned = seqinsertgaps(hk01_cds,al(1,:))
vt04_aligned = seqinsertgaps(vt04_cds,al(3,:))
```

5 Estimate the synonymous and nonsynonymous substitutions rates of the codon-aligned nucleotide sequences and also display the codons considered in the computations and their amino acid translations.

```
[dn,ds] = dndsml(hk01_aligned,vt04_aligned,'verbose',true)
```

References

[1] Tamura, K., and Mei, M. (1993). Estimation of the number of nucleotide substitutions in the control region of mitochondrial DNA in humans and chimpanzees. Molecular Biology and Evolution *10*, 512–526.

[2] Yang, Z., and Nielsen, R. (2000). Estimating synonymous and nonsynonymous substitution rates under realistic evolutionary models. Molecular Biology and Evolution *17*, 32–43.

See Also

Bioinformatics Toolbox functions: dnds, featuresparse, geneticcode, nt2aa, nwalign, seqinsertgaps, seqpdist

emblread

Purpose

Read data from EMBL file

Syntax

```
EMBLData = emblread('File')
EMBLSeq = emblread ('File', SequenceOnly',
SequenceOnlyValue)
```

Arguments

File	EMBL formatted file (ASCII text file). Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text for a file name.
SequenceOnlyValue	Property to control reading EMBL file information. If *SequenceOnlyValue* is `true`, `emblread` returns only the sequence (*EMBLSeq*).
EMBLData	MATLAB structure with fields corresponding to EMBL data.
EMBLSeq	MATLAB character string without metadata for the sequence.

Description

EMBLData = `emblread('`*File*`')` reads data from an EMBL formatted file (*File*) and creates a MATLAB structure (*EMBLData*) with fields corresponding to the EMBL two-character line type code. Each line type code is stored as a separate element in the structure.

EMBLData contains the following fields:

Field
`Identification.EntryName`
`Identification.Version`
`Identification.Topology`
`Identification.Molecule`
`Identification.DataClass`

Field
Identification.Division
Identification.SequenceLength
Accession
SequenceVersion
DateCreated
DateUpdated
Description
Keyword
OrganismSpecies
OrganismClassification
Organelle
Reference{#}.Number
Reference{#}.Comment
Reference{#}.Position
Reference{#}.MedLine
Reference{#}.PubMed
Reference{#}.Authors
Reference{#}.Title
Reference{#}.Location
DatabaseCrossReference
Comments
Feature
Basecount.BP
Basecount.A
Basecount.C

Field
`Basecount.G`
`Basecount.T`
`Basecount.Other`
`Sequence`

Note Topology information was not included in EMBL flat files before release 87 of the database. When reading a file created before release 87, EMBLREAD returns an empty Identification.Topology field.

Note The entry name is no longer displayed in the ID line of EMBL flat files in release 87. When reading a file created in release 87, EMBLREAD returns the accession number in the Identification.EntryName field.

`EMBLSeq = emblread ('File', SequenceOnly', SequenceOnlyValue)`, when *`SequenceOnlyValue`* is `true`, reads only the sequence information.

Examples

Get sequence information from the Web, save to a file, and then read back into MATLAB.

```
getembl('X00558','ToFile','rat_protein.txt');
EMBLData = emblread('rat_protein.txt')
```

See Also

Bioinformatics Toolbox functions: `fastaread`, `genbankread`, `getembl`, `seqtool`

evalrasmolscript

Purpose

Send RasMol script commands to Molecule Viewer window

Syntax

```
evalrasmolscript(FigureHandle, Command)
evalrasmolscript(FigureHandle, 'File', FileValue)
```

Arguments

FigureHandle	Figure handle to a molecule viewer returned by the `molviewer` function.
Command	Either of the following: • String specifying one or more RasMol script commands. Use a `;` to separate commands. • Character array or cell array containing strings specifying RasMol script commands. **Note** For a complete list of RasMol script commands, see `http://www.stolaf.edu/academics/chemapps/jmol/docs/`
FileValue	String specifying a file name or a path and file name of a text file containing Jmol script commands. If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Directory.

Description

`evalrasmolscript(`*`FigureHandle`*`, `*`Command`*`)` sends the RasMol script commands specified by *`Command`* to *`FigureHandle`*, the figure handle of a Molecule Viewer window created using the `molviewer` function.

`evalrasmolscript(`*`FigureHandle`*`, 'File', `*`FileValue`*`)` sends the RasMol script commands specified by *`FileValue`* to *`FigureHandle`*, the figure handle of a Molecule Viewer window created using the molviewer function.

Examples

1 Use the molviewer function to create a figure handle to a Molecule Viewer window.

```
FH = molviewer('2DHB')
```

2 Use the evalrasmolscript function to send script commands to the molecule viewer that change the background to black and spin the molecule.

```
evalrasmolscript(FH, 'background white; spin')
```

See Also

Bioinformatics Toolbox functions: getpdb, molviewer, pdbread, pdbwrite

Purpose

Calculate range of gene expression profiles

Syntax

```
Range = exprprofrange(Data)
[Range, LogRange] = exprprofrange(Data)
exprprofrange(..., 'PropertyName', PropertyValue,...)
exprprofrange(..., 'ShowHist', ShowHistValue)
```

Arguments

Data	Matrix where each row corresponds to a gene.
ShowHistValue	Property to control displaying a histogram with range data. Enter either `true` (include range data) or `false`. The default value is `false`.

Description

`Range = exprprofrange(Data)` calculates the range of each expression profile in a data set (*Data*).

`[Range, LogRange] = exprprofrange(Data)` returns the log range, that is, `log(max(prof))- log(min(prof))`, of each expression profile. If you do not specify output arguments, `exprprofrange` displays a histogram bar plot of the range.

`exprprofrange(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`exprprofrange(..., 'ShowHist', ShowHistValue)`, when *ShowHistValue* is `true`, displays a histogram of the range data.

Examples

Calculate the range of expression profiles for yeast data as gene expression changes during the metabolic shift from fermentation to respiration.

```
load yeastdata
range = exprprofrange(yeastvalues,'ShowHist',true);
```

See Also

Bioinformatics Toolbox function `exprprofvar`, `generangefilter`

exprprofvar

Purpose

Calculate variance of gene expression profiles

Syntax

```
Variance = exprprofvar(Data)
exprprofvar(..., 'PropertyName', PropertyValue,...)
exprprofvar(..., 'ShowHist', ShowHistValue)
```

Arguments

Data	Matrix where each row corresponds to a gene.
ShowHistValue	Property to control the display of a histogram with variance data. Enter either `true` or `false` (default).

Description

Variance = `exprprofvar(`*Data*`)` calculates the variance of each expression profile in a data set (*Data*). If you do not specify output arguments, this function displays a histogram bar plot of the range.

`exprprofvar(..., '`*PropertyName*`', `*PropertyValue*`,...)` defines optional properties using property name/value pairs.

`exprprofvar(..., 'ShowHist', `*ShowHistValue*`)`, when `ShowHist` is `true`, displays a histogram of the range data .

Examples

Calculate the variance of expression profiles for yeast data as gene expression changes during the metabolic shift from fermentation to respiration.

```
load yeastdata
datavar = exprprofvar(yeastvalues,'ShowHist',true);
```

See Also

Bioinformatics Toolbox functions `exprprofrange`, `generangefilter`, `genevarfilter`

Purpose

Read data from FASTA file

Syntax

```
FASTAData = fastaread(File)
[Header, Sequence] = fastaread(File)
fastaread(..., 'PropertyName', PropertyValue, ...)
fastaread(..., 'IgnoreGaps', IgnoreGapsValue, ...)
fastaread(..., 'Blockread', BlockreadValue, ...)
```

Arguments

File	FASTA-formatted file (ASCII text file). Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text for a file name.
FASTAData	MATLAB structure with the fields `Header` and `Sequence`.
IgnoreGapsValue	Property to control removing gap symbols. Enter either `true` or `false` (default).
BlockreadValue	Property to control reading a single entry or block of entries from a file containing multiple sequences. Enter a scalar `N`, to read the `N`th entry in the file. Enter a 1-by-2 vector [*M1, M2*], to read the block of entries starting at entry *M1* and ending at entry *M2*. To read all remaining entries in the file starting at entry *M1*, enter a positive value for *M1* and enter `Inf` for *M2*.

Description

`fastaread` reads data from a FASTA-formatted file into a MATLAB structure with the following fields:

Field
Header
Sequence

A file with a FASTA format begins with a right angle bracket (>) and a single line description. Following this description is the sequence as a series of lines with fewer than 80 characters. Sequences are expected to use the standard IUB/IUPAC amino acid and nucleotide letter codes.

For a list of codes, see `aminolookup` and `baselookup`.

`*FASTAData* = fastaread(*File*)` reads a file with a FASTA format and returns the data in a structure. `FASTAData.Header` is the header information, while `FASTAData.Sequence` is the sequence stored as a string of letters.

`[*Header, Sequence*] = fastaread(*File*)` reads data from a file into separate variables. If the file contains more than one sequence, then `header` and `sequence` are cell arrays of header and sequence information.

`fastaread(..., '*PropertyName*', *PropertyValue*, ...)`defines optional properties. The property name/value pairs can be in any format supported by the function `set` (for example, name-value string pairs, structures, and name-value cell array pairs).

`fastaread(..., 'IgnoreGaps', *IgnoreGapsValue*, ...)`, when *`IgnoreGapsValue`* is `true`, removes any gap symbol (`'-'` or `'.'`) from the sequences. Default is `false`.

`fastaread(..., 'Blockread', *BlockreadValue*, ...)` lets you read in a single entry or block of entries from a file containing multiple sequences. If *`BlockreadValue`* is a scalar `N`, then `fastaread` reads the `N`th entry in the file. If *`BlockreadValue`* is a 1-by-2 vector [*`M1, M2`*], then `fastaread` reads the block of entries starting at entry *`M1`* and ending at entry *`M2`*. To read all remaining entries in the file starting at entry *`M1`*, enter a positive value for *`M1`* and enter `Inf` for *`M2`*.

Examples

Read the sequence for the human p53 tumor gene.

```
p53nt = fastaread('p53nt.txt')
```

Read the sequence for the human p53 tumor protein.

```
p53aa = fastaread('p53aa.txt')
```

Read the human mitochondrion genome in FASTA format.

```
entrezSite = 'http://www.ncbi.nlm.nih.gov/entrez/viewer.fcgi?'
textOptions = '&txt=on&view=fasta'
genbankID = '&list_uids=NC_001807'
mitochondrion = fastaread([entrezSite textOptions genbankID])
```

See Also

Bioinformatics Toolbox functions: `emblread`, `fastawrite`, `genbankread`, `genpeptread`, `multialignread`, `seqprofile`, `seqtool`

fastawrite

Purpose

Write to file using FASTA format

Syntax

```
fastawrite(File, Data)
fastawrite(File, Header, Sequence)
```

Arguments

File	String specifying either a file name or a path and file name supported by your operating system. If you specify only a file name, the file is saved to the MATLAB Current Directory.
Data	Any of the following: • String with a FASTA format • Sequence object • MATLAB structure containing the fields `Header` and `Sequence` • GenBank/GenPept structure
Header	String containing information about the sequence. This text will be included in the header of the FASTA-formatted file, *File*.
Sequence	String or name of variable containing an amino acid or nucleotide sequence using the standard IUB/IUPAC letter or integer codes. For a list of valid characters, see Amino Acid Lookup Table on page 2-42 or Nucleotide Lookup Table on page 2-52.

Description

`fastawrite(`*File*`,` *Data*`)` writes the contents of *Data* to a FASTA-formatted file (ASCII text file).

`fastawrite(`*File*`,` *Header*`,` *Sequence*`)` writes the specified header and sequence information to a FASTA-formatted file (ASCII text file).

Examples

```
%get the sequence for the human p53 gene from GenBank.
seq = getgenbank('NM_000546')
```

```
%find the CDS line in the FEATURES information.
cdsline = strmatch('CDS',seq.Features)

%read the coordinates of the coding region.
[start,stop] = strread(seq.Features(cdsline,:),'%*s%d..%d')

%extract the coding region.
codingSeq = seq.Sequence(start:stop)

%write just the coding region to a FASTA file.
fastawrite('p53coding.txt','Coding region for p53',codingSeq);
```

Save multiple sequences.

```
data(1).Sequence = 'ACACAGGAAA'
data(1).Header = 'First sequence'
data(2).Sequence = 'ACGTCAGGTC'
data(2).Header = 'Second sequence'

fastawrite('my_sequences.txt', data)
type('my_sequences.txt')

>First sequence
ACACAGGAAA

>Second sequence
ACGTCAGGTC
```

See Also

Bioinformatics Toolbox functions: `fastaread`, `seqtool`

featuresmap

Purpose Draw linear or circular map of features from GenBank structure

Syntax

```
featuresmap(GBStructure)
featuresmap(GBStructure, FeatList)
featuresmap(GBStructure, FeatList, Levels)
featuresmap(GBStructure, Levels)
[Handles, OutFeatList] = featuresmap(...)
featuresmap(..., 'FontSize', FontSizeValue, ...)
featuresmap(..., 'ColorMap', ColorMapValue, ...)
featuresmap(..., 'Qualifiers', QualifiersValue, ...)
featuresmap(..., 'ShowPositions', ShowPositionsValue, ...)
```

Arguments

GBStructure — GenBank structure, typically created using the `getgenbank` or the `genbankread` function.

FeatList — Cell array of features (from the list of all features in the GenBank structure) to include in or exclude from the map.

- If *FeatList* is a cell array of features, these features are mapped. Any features in *FeatList* not found in the GenBank structure are ignored.
- If *FeatList* includes `'-'` as the first string in the cell array, then the remaining strings (features) are not mapped.

By default, *FeatList* is the a list of all features in the GenBank structure.

Levels	Vector of N integers, where N is the number of features. Each integer represents the level in the map for the corresponding feature. For example, if *Levels* = [1, 1, 2, 3, 3], the first two features would appear on level 1, the third feature on level 2, and the fourth and fifth features on level 3. By default, *Levels* = [1:N].
FontSizeValue	Scalar that sets the font size (points) for the annotations of the features. Default is 9.
ColorMapValue	Three-column matrix, to specify a list of colors to use for each feature. This matrix replaces the default matrix, which specifies the following colors and order: blue, green, red, cyan, magenta, yellow, brown, light green, orange, purple, gold, and silver. In the matrix, each row corresponds to a color, and each column specifies red, green, and blue intensity respectively. Valid values for the RGB intensities are 0.0 to 1.0.

QualifiersValue	Cell array of strings to specify an ordered list of qualifiers to search for in the structure and use as annotations. For each feature, the first matching qualifier found from the list is used for its annotation. If a feature does not include any of the qualifiers, no annotation displays for that feature. By default, *QualifiersValue* = {'*gene*', '*product*', '*locus_tag*', '*note*', '*db_xref*', '*protein_id*'}. Provide your own *QualifiersValue* to limit or expand the list of qualifiers or change the search order.

Tip Set *QualifiersValue* = {} to create a map with no annotations.

Tip To determine all qualifiers available for a given feature, do either of the following:

- Create the map, and then click a feature or its annotation to list all qualifiers for that feature.
- Use the `featuresparse` command to parse all the features into a new structure, and then use the `fieldnames` command to list the qualifiers for a specific feature. See Determining Qualifiers for a Specific Feature on page 2-150.

ShowPositionsValue	Property to add the sequence position to the annotation label for each feature. Enter `true` to add the sequence position. Default is `false`.

Description

featuresmap(*GBStructure*) creates a linear or circular map of all features from a GenBank structure, typically created using the getgenbank or the genbankread function.

featuresmap(*GBStructure*, *FeatList*) creates a linear or circular map of a subset of features from a GenBank structure. *FeatList* lets you specify features (from the list of all features in the GenBank structure) to include in or exclude from the map.

- If *FeatList* is a cell array of features, these features are mapped. Any features in *FeatList* not found in the GenBank structure are ignored.
- If *FeatList* includes '-' as the first string in the cell array, then the remaining strings (features) are not mapped.

By default, *FeatList* is a list of all features in the GenBank structure.

featuresmap(*GBStructure*, *FeatList*, *Levels*) or featuresmap(*GBStructure*, *Levels*) indicates which level on the map each feature is drawn. Level 1 is the left-most (linear map) or inner-most (circular map) level, and level N is the right-most (linear map) or outer-most (circular map) level, where N is the number of features.

Levels is a vector of N integers, where N is the number of features. Each integer represents the level in the map for the corresponding feature. For example, if *Levels* = [1, 1, 2, 3, 3], the first two features would appear on level 1, the third feature on level 2, and the fourth and fifth features on level 3. By default, *Levels* = [1:N].

[*Handles, OutFeatList*] = featuresmap(...) returns a list of handles for each feature in *OutFeatList*. It also returns *OutFeatList*, which is a cell array of the mapped features.

Tip Use *Handles* and *OutFeatList* with the legend command to create a legend of features.

`featuresmap(..., 'PropertyName', PropertyValue, ...)` defines optional properties that use property name/value pairs in any order. These property name/value pairs are as follows:

`featuresmap(..., 'FontSize', FontSizeValue, ...)` sets the font size (points) for the annotations of the features. Default *`FontSizeValue`* is `9`.

`featuresmap(..., 'ColorMap', ColorMapValue, ...)` specifies a list of colors to use for each feature. This matrix replaces the default matrix, which specifies the following colors and order: blue, green, red, cyan, magenta, yellow, brown, light green, orange, purple, gold, and silver. *`ColorMapValue`* is a three-column matrix, where each row corresponds to a color, and each column specifies red, green, and blue intensity respectively. Valid values for the RGB intensities are `0.0` to `1.0`.

`featuresmap(..., 'Qualifiers', QualifiersValue, ...)` lets you specify an ordered list of qualifiers to search for and use as annotations. For each feature, the first matching qualifier found from the list is used for its annotation. If a feature does not include any of the qualifiers, no annotation displays for that feature. *`QualifiersValue`* is a cell array of strings. By default, `QualifiersValue = {'gene', 'product', 'locus_tag', 'note', 'db_xref', 'protein_id'}`. Provide your own *`QualifiersValue`* to limit or expand the list of qualifiers or change the search order.

Tip Set `QualifiersValue = {}` to create a map with no annotations.

Tip To determine all qualifiers available for a given feature, do either of the following:

- Create the map, and then click a feature or its annotation to list all qualifiers for that feature.
- Use the `featuresparse` command to parse all the features into a new structure, and then use the `fieldnames` command to list the qualifiers for a specific feature. See Determining Qualifiers for a Specific Feature on page 2-150.

`featuresmap(..., 'ShowPositions', ShowPositionsValue, ...)` lets you add the sequence position to the annotation label. If *`ShowPositionsValue`* is `true`, sequence positions are added to the annotation labels. Default is `false`.

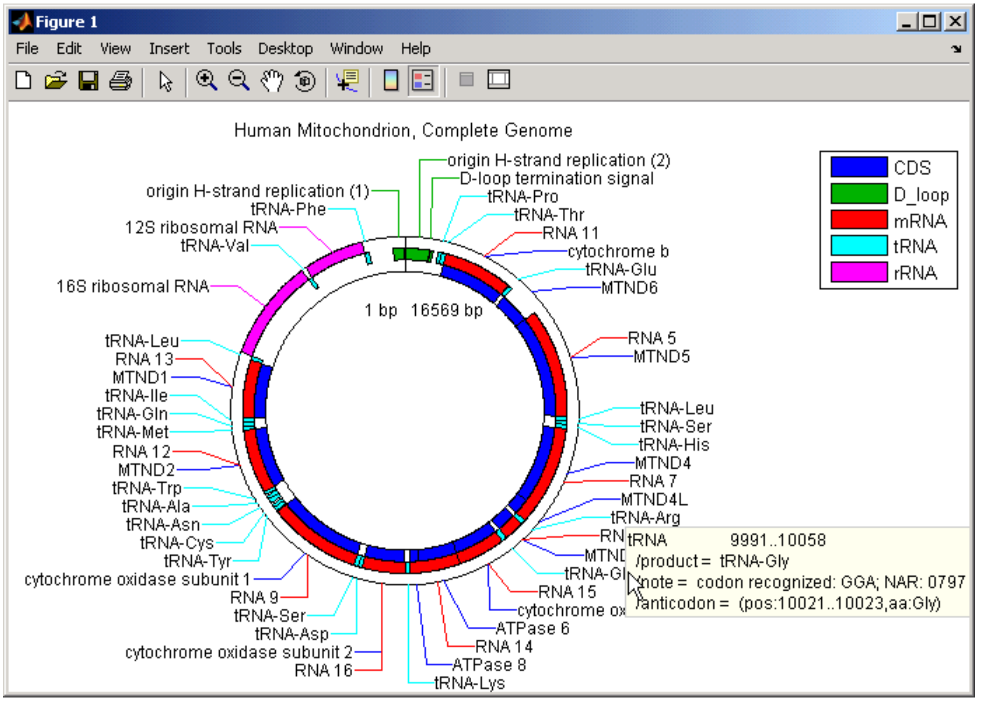


Figure 1
File Edit View Insert Tools Desktop Window Help
Human Mitochondrion, Complete Genome
CDS
D_loop
mRNA
tRNA
rRNA
1 bp 16569 bp
origin H-strand replication (2)
D-loop termination signal
tRNA-Pro
tRNA-Thr
RNA 11
cytochrome b
tRNA-Glu
MTND6
RNA 5
MTND5
tRNA-Leu
tRNA-Ser
tRNA-His
MTND4
RNA 7
MTND4L
tRNA-Arg
RNA 15
ATPase 6
RNA 14
ATPase 8
tRNA-Lys
RNA 16
cytochrome oxidase subunit 2
tRNA-Asp
tRNA-Ser
RNA 9
cytochrome oxidase subunit 1
tRNA-Tyr
tRNA-Cys
tRNA-Asn
tRNA-Ala
tRNA-Trp
MTND2
RNA 12
tRNA-Met
tRNA-Gln
tRNA-Ile
MTND1
RNA 13
tRNA-Leu
16S ribosomal RNA
tRNA-Val
12S ribosomal RNA
tRNA-Phe
origin H-strand replication (1)
tRNA 9991..10058
/product = tRNA-Gly
/note = codon recognized: GGA; NAR: 0797
/anticodon = (pos:10021..10023,aa:Gly)

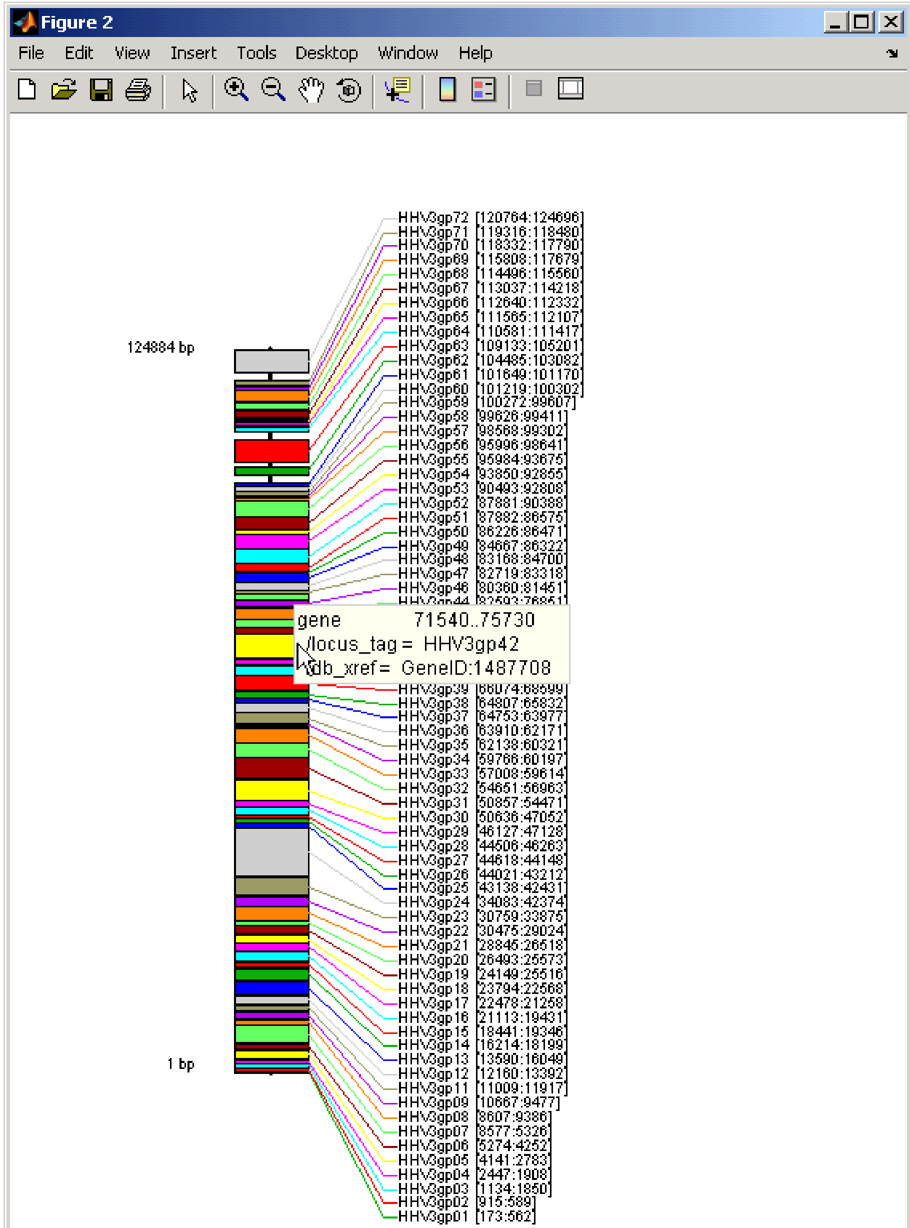


Figure 2
File Edit View Insert Tools Desktop Window Help
124884 bp
1 bp
HHV3gp72 [120764:124696]
HHV3gp71 [119316:118480]
HHV3gp70 [118332:117790]
HHV3gp69 [115808:117679]
HHV3gp68 [114496:115560]
HHV3gp67 [113037:114218]
HHV3gp66 [112640:112332]
HHV3gp65 [111565:112107]
HHV3gp64 [110581:111417]
HHV3gp63 [109133:105201]
HHV3gp62 [104485:103082]
HHV3gp61 [101649:101170]
HHV3gp60 [101219:100302]
HHV3gp59 [100272:99607]
HHV3gp58 [99626:99411]
HHV3gp57 [98568:99302]
HHV3gp56 [95996:98641]
HHV3gp55 [95984:93675]
HHV3gp54 [93850:92855]
HHV3gp53 [90493:92808]
HHV3gp52 [87881:90388]
HHV3gp51 [87882:86575]
HHV3gp50 [86226:86471]
HHV3gp49 [84667:86322]
HHV3gp48 [83168:84700]
HHV3gp47 [82719:83318]
HHV3gp46 [80360:81451]
gene 71540..75730
locus_tag = HHV3gp42
db_xref = GeneID:1487708
HHV3gp38 [64807:65832]
HHV3gp37 [64753:63977]
HHV3gp36 [63910:62171]
HHV3gp35 [62138:60321]
HHV3gp34 [59766:60197]
HHV3gp33 [57008:59614]
HHV3gp32 [54651:56963]
HHV3gp31 [50857:54471]
HHV3gp30 [50636:47052]
HHV3gp29 [46127:47128]
HHV3gp28 [44506:46263]
HHV3gp27 [44618:44148]
HHV3gp26 [44021:43212]
HHV3gp25 [43138:42431]
HHV3gp24 [34083:42374]
HHV3gp23 [30759:33875]
HHV3gp22 [30475:29024]
HHV3gp21 [28845:26518]
HHV3gp20 [26493:25573]
HHV3gp19 [24149:25516]
HHV3gp18 [23794:22568]
HHV3gp17 [22478:21258]
HHV3gp16 [21113:19431]
HHV3gp15 [18441:19346]
HHV3gp14 [16214:18199]
HHV3gp13 [13590:16049]
HHV3gp12 [12160:13392]
HHV3gp11 [11009:11917]
HHV3gp09 [10667:9477]
HHV3gp08 [8607:9386]
HHV3gp07 [8577:5326]
HHV3gp06 [5274:4252]
HHV3gp05 [4141:2783]
HHV3gp04 [2447:1908]
HHV3gp03 [1134:1850]
HHV3gp02 [915:589]
HHV3gp01 [173:562]

After creating a map:

- Click a feature or annotation to display a list of all qualifiers for that feature.
- Zoom the plot by clicking the following buttons:

   or 

Examples

Creating a Circular Map with Legend

The following example creates a circular map of five different features mapped on three levels. It also uses outputs from the `featuresmap` function as inputs to the `legend` function to add a legend to the map.

```
GBStructure = getgenbank('J01415');
[Handles, OutFeatList] = featuresmap(GBStructure, ...
     {'CDS','D_loop','mRNA','tRNA','rRNA'}, [1 2 2 2 3])
legend(Handles, OutFeatList, 'interpreter', 'none', ...
     'location','bestoutside')
title('Human Mitochondrion, Complete Genome')
```

Creating a Linear Map with Sequence Position Labels and Changed Font Size

The following example creates a linear map showing only the gene feature. It changes the font of the labels to seven points and includes the sequence position in the labels.

```
herpes = getgenbank('NC_001348');
featuresmap(herpes,{'gene'},'fontsize',7,'showpositions',true)
title('Genes in Human herpesvirus 3 (strain Dumas)')
```

Determining Qualifiers for a Specific Feature

The following example uses the `getgenbank` function to create a GenBank structure, `GBStructure`. It then uses the `featuresparse` function to parse the features in the GenBank structure into a new structure, `features`. It then uses the `fieldnames` function to return all qualifiers for one of the features, `D_loop`.

```
GenBankStructure = getgenbank('J01415');
features = featuresparse (GenBankStructure)
features =

         source: [1x1 struct]
         D_loop: [1x2 struct]
     rep_origin: [1x3 struct]
    repeat_unit: [1x4 struct]
    misc_signal: [1x1 struct]
       misc_RNA: [1x1 struct]
      variation: [1x17 struct]
           tRNA: [1x22 struct]
           rRNA: [1x2 struct]
           mRNA: [1x10 struct]
            CDS: [1x13 struct]
       conflict: [1x1 struct]

fieldnames(features.D_loop)

ans =

    'Location'
    'Indices'
    'note'
    'citation'
```

See Also

`featuresparse`, `genbankread`, `getgenbank`, `seqtool`

featuresparse

Purpose

Parse features from GenBank, GenPept, or EMBL data

Syntax

```
FeatStruct = featuresparse(Features)
FeatStruct = featuresparse(Features, ...'Feature',
FeatureValue, ...)
FeatStruct = featuresparse(Features, ...'Sequence',
   SequenceValue, ...)
```

Arguments

Features	Any of the following: • String containing GenBank, GenPept, or EMBL features • MATLAB character array including text describing GenBank, GenPept, or EMBL features • MATLAB structure with fields corresponding to GenBank, GenPept, or EMBL data, such as those returned by `genbankread`, `genpeptread`, `emblread`, `getgenbank`, `getgenpept`, or `getembl`
FeatureValue	Name of a feature contained in *Features*. When specified, `featuresparse` returns only the substructure that corresponds to this feature. If there are multiple features with the same *FeatureValue*, then *FeatStruct* is an array of structures.
SequenceValue	Property to control the extraction, when possible, of the sequences respective to each feature, joining and complementing pieces of the source sequence and storing them in the `Sequence` field of the returned structure, *FeatStruct*. When extracting the sequence from an incomplete CDS feature, `featuresparse` uses the `codon_start` qualifier to adjust the frame of the sequence. Choices are `true` or `false` (default).

Return Values

FeatStruct	Output structure containing a field for every database feature. Each field name in *FeatStruct* matches the corresponding feature name in the GenBank, GenPept, or EMBL database, with the exceptions listed in the table below. Fields in *FeatStruct* contain substructures with feature qualifiers as fields. In the GenBank, GenPept, and EMBL databases, for each feature, the only mandatory qualifier is its location, which `featuresparse` translates to the field `Location`. When possible, `featuresparse` also translates this location to numeric indices, creating an `Indices` field.

Note If you use the `Indices` field to extract sequence information, you may need to complement the sequences.

Description

`FeatStruct = featuresparse(Features)` parses the features from *Features*, which contains GenBank, GenPept, or EMBL features. *Features* can be a:

- String containing GenBank, GenPept, or EMBL features
- MATLAB character array including text describing GenBank, GenPept, or EMBL features
- MATLAB structure with fields corresponding to GenBank, GenPept, or EMBL data, such as those returned by `genbankread`, `genpeptread`, `emblread`, `getgenbank`, `getgenpept`, or `getembl`

FeatStruct is the output structure containing a field for every database feature. Each field name in *FeatStruct* matches the corresponding feature name in the GenBank, GenPept, or EMBL database, with the following exceptions.

Feature Name in GenBank, GenPept, or EMBL Database	Field Name in MATLAB Structure
`-10_signal`	`minus_10_signal`
`-35_signal`	`minus_35_signal`
`3'UTR`	`three_prime_UTR`
`3'clip`	`three_prime_clip`
`5'UTR`	`five_prime_UTR`
`5'clip`	`five_prime_clip`
`D-loop`	`D_loop`

Fields in *`FeatStruct`* contain substructures with feature qualifiers as fields. In the GenBank, GenPept, and EMBL databases, for each feature, the only mandatory qualifier is its location, which `featuresparse` translates to the field `Location`. When possible, `featuresparse` also translates this location to numeric indices, creating an `Indices` field.

Note If you use the `Indices` field to extract sequence information, you may need to complement the sequences.

`FeatStruct` `= featuresparse (`*`Features`*`, ...'`*`PropertyName`*`',` *`PropertyValue`*`, ...)` calls `featuresparse` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`FeatStruct` `= featuresparse(`*`Features`*`, ...'Feature',` *`FeatureValue`*`, ...)` returns only the substructure that corresponds to *`FeatureValue`*, the name of a feature contained in *`Features`*. If there are multiple

features with the same *FeatureValue*, then *FeatStruct* is an array of structures.

FeatStruct = featuresparse(*Features*, ...'Sequence', *SequenceValue*, ...) controls the extraction, when possible, of the sequences respective to each feature, joining and complementing pieces of the source sequence and storing them in the field Sequence. When extracting the sequence from an incomplete CDS feature, featuresparse uses the codon_start qualifier to adjust the frame of the sequence. Choices are true or false (default).

Examples

Obtaining All Features from a GenBank File

The following example obtains all the features stored in the GenBank file nm175642.txt:

```
gbkStruct = genbankread('nm175642.txt');
features = featuresparse(gbkStruct)

features =

    source: [1x1 struct]
      gene: [1x1 struct]
       CDS: [1x1 struct]
```

Obtaining a Subset of Features from a GenBank Record

The following example obtains only the coding sequences (CDS) feature of the *Caenorhabditis elegans* cosmid record (accession number Z92777) from the GenBank database:

```
worm = getgenbank('Z92777');
CDS = featuresparse(worm,'feature','cds')

CDS =

1x12 struct array with fields:
    Location
    Indices
```

```
locus_tag
standard_name
note
codon_start
product
protein_id
db_xref
translation
```

Extracting Sequences for Each Feature

1 Retrieve two nucleotide sequences from the GenBank database for the neuraminidase (NA) protein of two strains of the Influenza A virus (H5N1).

```
hk01 = getgenbank('AF509094');
vt04 = getgenbank('DQ094287');
```

2 Extract the sequence of the coding region for the neuraminidase (NA) protein from the two nucleotide sequences. The sequences of the coding regions are stored in the `Sequence` fields of the returned structures, `hk01_cds` and `vt04_cds`.

```
hk01_cds = featuresparse(hk01,'feature','CDS','Sequence',true);
vt04_cds = featuresparse(vt04,'feature','CDS','Sequence',true);
```

3 Once you have extracted the nucleotide sequences, you can use the `nt2aa` and `nwalign` functions to align the amino acids sequences converted from the nucleotide sequences.

```
[sc,al]=nwalign(nt2aa(hk01_cds),nt2aa(vt04_cds),'extendgap',1);
```

4 Then you can use the `seqinsertgaps` function to copy the gaps from the aligned amino acid sequences to their corresponding nucleotide sequences, thus codon-aligning them.

```
hk01_aligned = seqinsertgaps(hk01_cds,al(1,:))
vt04_aligned = seqinsertgaps(vt04_cds,al(3,:))
```

5 Once you have code aligned the two sequences, you can use them as input to other functions such as `dnds`, which calculates the synonymous and nonsynonymous substitutions rates of the codon-aligned nucleotide sequences. By setting `Verbose` to `true`, you can also display the codons considered in the computations and their amino acid translations.

```
[dn,ds] = dnds(hk01_aligned,vt04_aligned,'verbose',true)
```

See Also

Bioinformatics Toolbox functions: `emblread`, `genbankread`, `genpeptread`, `getgenbank`, `getgenpept`

galread

Purpose

Read microarray data from GenePix array list file

Syntax

```
GALData = galread('File')
```

Arguments

File	GenePix Array List formatted file (GAL). Enter a file name, or enter a path and file name.

Description

`galread` reads data from a GenePix formatted file into a MATLAB structure.

GALData = `galread('`*File*`')` reads in a GenePix Array List formatted file (*File*) and creates a structure (`GALData`) containing the following fields:

Field
`Header`
`BlockData`
`IDs`
`Names`

The field `BlockData` is an `N`-by-`3` array. The columns of this array are the block data, the column data, and the row data respectively. For more information on the GAL format, see

```
http://www.moleculardevices.com/pages/software/gn_genepix_file_formats.html#gal
```

For a list of supported file format versions, see

```
http://www.moleculardevices.com/pages/software/gn_genepix_file_formats.html
```

GenePix is a registered trademark of Molecular Devices Corporation.

See Also

Bioinformatics Toolbox functions: `affyread`, `geosoftread`, `gprread`, `imageneread`, `sptread`

Purpose

Perform GC Robust Multi-array Average (GCRMA) background adjustment, quantile normalization, and median-polish summarization on Affymetrix microarray probe-level data

Syntax

```
ExpressionMatrix = gcrma(PMMatrix, MMMatrix, ProbeIndices,
   AffinPM, AffinMM)
ExpressionMatrix = gcrma(PMMatrix, MMMatrix, ProbeIndices,
   SequenceMatrix)
ExpressionMatrix = gcrma( ...'ChipIndex',
ChipIndexValue, ...)
ExpressionMatrix = gcrma( ...'OpticalCorr',
OpticalCorrValue,
   ...)
ExpressionMatrix = gcrma( ...'CorrConst', CorrConstValue,
   ...)
ExpressionMatrix = gcrma( ...'Method', MethodValue, ...)
ExpressionMatrix = gcrma( ...'TuningParam',
TuningParamValue,
   ...)
ExpressionMatrix = gcrma( ...'GSBCorr', GSBCorrValue, ...)
ExpressionMatrix = gcrma( ...'Normalize', NormalizeValue,
   ...)
ExpressionMatrix = gcrma( ...'Verbose', VerboseValue, ...)
```

Arguments

PMMatrix

Matrix of intensity values where each row corresponds to a perfect match (PM) probe and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)

Tip You can use the `PMIntensities` matrix returned by the `celintensityread` function.

MMMatrix

Matrix of intensity values where each row corresponds to a mismatch (MM) probe and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)

Tip You can use the `MMIntensities` matrix returned by the `celintensityread` function.

ProbeIndices

Column vector containing probe indices. Probes within a probe set are numbered 0 through N - 1, where N is the number of probes in the probe set.

Tip You can use the `affyprobeseqread` function to generate this column vector.

AffinPM	Column vector of PM probe affinities.

Tip You can use the `affyprobeaffinities` function to generate this column vector.

AffinMM	Column vector of MM probe affinities.

Tip You can use the `affyprobeaffinities` function to generate this column vector.

SequenceMatrix	An *N*-by-25 matrix of sequence information for the perfect match (PM) probes on the Affymetrix GeneChip array, where *N* is the number of probes on the array. Each row corresponds to a probe, and each column corresponds to one of the 25 sequence positions. Nucleotides in the sequences are represented by one of the following integers: • `0` — None • `1` — A • `2` — C • `3` — G • `4` — T **Tip** You can use the `affyprobeseqread` function to generate this matrix. If you have this sequence information in letter representation, you can convert it to integer representation using the `nt2int` function.
ChipIndexValue	Positive integer specifying a column index in *MMMatrix*, which specifies a chip. This chip intensity data is used to compute probe affinities, assuming no affinity data is provided. Default is `1`.
OpticalCorrValue	Controls the use of optical background correction on the PM and MM intensity values in *PMMatrix* and *MMMatrix*. Choices are `true` (default) or `false`.

CorrConstValue	Value that specifies the correlation constant, rho, for background intensity for each PM/MM probe pair. Choices are any value ≥ `0` and ≤ `1`. Default is `0.7`.
MethodValue	String that specifies the method to estimate the signal. Choices are `MLE`, a faster, ad hoc Maximum Likelihood Estimate method, or `EB`, a slower, more formal, empirical Bayes method. Default is `MLE`.
TuningParamValue	Value that specifies the tuning parameter used by the estimate method. This tuning parameter sets the lower bound of signal values with positive probability. Choices are a positive value. Default is `5` (MLE) or `0.5` (EB). **Tip** For information on determining a setting for this parameter, see Wu et al., 2004.
GSBCorrValue	Controls whether gene specific binding (GSB) correction is performed on the non-specific binding (NSB) data. Choices are `true` (default) or `false`.
NormalizeValue	Controls whether quantile normalization is performed on background adjusted data. Choices are `true` (default) or `false`.
VerboseValue	Controls the display of a progress report showing the number of each chip as it is completed. Choices are `true` (default) or `false`.

Return Values

ExpressionMatrix Matrix of $\log_2$ expression values where each row corresponds to a gene (probe set) and each column corresponds to an Affymetrix CEL file, which represents a single chip.

Description

`ExpressionMatrix = gcrma(PMMatrix, MMMatrix, ProbeIndices, AffinPM, AffinMM)` performs GCRMA background adjustment, quantile normalization , and median-polish summarization on Affymetrix microarray probe-level data using probe affinity data. *ExpressionMatrix* is a matrix of $\log_2$ expression values where each row corresponds to a gene (probe set) and each column corresponds to an Affymetrix CEL file, which represents a single chip.

Note There is no column in *ExpressionMatrix* that contains probe set or gene information.

`ExpressionMatrix = gcrma(PMMatrix, MMMatrix, ProbeIndices, SequenceMatrix)` performs GCRMA background adjustment, quantile normalization, and Robust Multi-array Average (RMA) summarization on Affymetrix microarray probe-level data using probe sequence data to compute probe affinity data. *ExpressionMatrix* is a matrix of $\log_2$ expression values where each row corresponds to a gene (probe set) and each column corresponds to an Affymetrix CEL file, which represents a single chip.

Note If *AffinPM* and *AffinMM* affinity data and *SequenceMatrix* sequence data are not available, you can still use the `gcrma` function by entering an empty matrix for these inputs in the syntax.

`ExpressionMatrix = gcrma( ...'PropertyName', PropertyValue, ...)` calls `gcrma` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

ExpressionMatrix = gcrma(...'ChipIndex', *ChipIndexValue*, ...) computes probe affinities from MM probe intensity data from the chip with the specified column index in *MMMatrix*, assuming no affinity data is provided. Default *ChipIndexValue* is 1. If *AffinPM* and *AffinMM* affinity data are provided, this property is ignored.

ExpressionMatrix = gcrma(...'OpticalCorr', *OpticalCorrValue*, ...) controls the use of optical background correction on the PM and MM intensity values in *PMMatrix* and *MMMatrix*. Choices are true (default) or false.

ExpressionMatrix = gcrma(...'CorrConst', *CorrConstValue*, ...) specifies the correlation constant, rho, for background intensity for each PM/MM probe pair. Choices are any value ≥ 0 and ≤ 1. Default is 0.7.

ExpressionMatrix = gcrma(...'Method', *MethodValue*, ...) specifies the method to estimate the signal. Choices are MLE, a faster, ad hoc Maximum Likelihood Estimate method, or EB, a slower, more formal, empirical Bayes method. Default is MLE.

ExpressionMatrix = gcrma(...'TuningParam', *TuningParamValue*, ...) specifies the tuning parameter used by the estimate method. This tuning parameter sets the lower bound of signal values with positive probability. Choices are a positive value. Default is 5 (MLE) or 0.5 (EB).

Tip For information on determining a setting for this parameter, see Wu et al., 2004.

ExpressionMatrix = gcrma(...'GSBCorr', *GSBCorrValue*, ...) controls whether gene specific binding (GSB) correction is performed on the non-specific binding (NSB) data. Choices are `true` (default) or `false`.

`ExpressionMatrix = gcrma( ...'Normalize', NormalizeValue, ...)` controls whether quantile normalization is performed on background adjusted data. Choices are `true` (default) or `false`.

`ExpressionMatrix = gcrma( ...'Verbose', VerboseValue, ...)` controls the display of a progress report showing the number of each chip as it is completed. Choices are `true` (default) or `false`.

Examples

1. Load the MAT file, included with Bioinformatics Toolbox, that contains Affymetrix data from a prostate cancer study. The variables in the MAT file include `seqMatrix`, a matrix containing sequence information for PM probes, `pmMatrix` and `mmMatrix`, matrices containing PM and MM probe intensity values, and `probeIndices`, a column vector containing probe indexing information.

```
load prostatecancerrawdata
```

2. Compute the Affymetrix PM and MM probe affinities from their sequences and MM probe intensities.

```
[apm, amm] = affyprobeaffinities(seqMatrix, mmMatrix(:,1),...
                                  'ProbeIndices', probeIndices);
```

3. Perform GCRMA background adjustment, quantile normalization, and Robust Multi-array Average (RMA) summarization on the Affymetrix microarray probe-level data and create a matrix of expression values.

```
expdata = gcrma(pmMatrix, mmMatrix, probeIndices, seqMatrix);
```

The `prostatecancerrawdata.mat` file used in this example contains data from Best et al., 2005.

References

[1] Wu, Z., Irizarry, R.A., Gentleman, R., Murillo, F.M. and Spencer, F. (2004). A Model Based Background Adjustment for Oligonucleotide

Expression Arrays. Journal of the American Statistical Association *99(468)*, 909–917.

[2] Wu, Z., and Irizarry, R.A. (2005). Stochastic Models Inspired by Hybridization Theory for Short Oligonucleotide Arrays. Proceedings of RECOMB 2004. J Comput Biol. *12(6)*, 882–93.

[3] Wu, Z., and Irizarry, R.A. (2005). A Statistical Framework for the Analysis of Microarray Probe-Level Data. Johns Hopkins University, Biostatistics Working Papers 73.

[4] Speed, T. (2006). Background models and GCRMA. Lecture 10, Statistics 246, University of California Berkeley. `http://www.stat.berkeley.edu/users/terry/Classes/s246.2006/Week10/Week`
.

[5] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

See Also

Bioinformatics Toolbox functions: `affyprobeseqread`, `affyread`, `celintensityread`, `gcrmabackadj`, `quantilenorm`, `rmabackadj`, `rmasummary`

gcrmabackadj

Purpose

Perform GC Robust Multi-array Average (GCRMA) background adjustment on Affymetrix microarray probe-level data using sequence information

Syntax

```
PMMatrix_Adj = gcrmabackadj(PMMatrix, MMMatrix, AffinPM,
   AffinMM)
[PMMatrix_Adj, nsbStruct] = gcrmabackadj(PMMatrix,
MMMatrix,
   AffinPM, AffinMM)
... = gcrmabackadj( ...'OpticalCorr',
OpticalCorrValue, ...)
... = gcrmabackadj( ...'CorrConst', CorrConstValue, ...)
... = gcrmabackadj( ...'Method', MethodValue, ...)
... = gcrmabackadj( ...'TuningParam',
TuningParamValue, ...)
... = gcrmabackadj( ...'AddVariance',
AddVarianceValue, ...)
... = gcrmabackadj( ...'Showplot', ShowplotValue, ...)
... = gcrmabackadj( ...'Verbose', VerboseValue, ...)
```

Arguments

PMMatrix
: Matrix of intensity values where each row corresponds to a perfect match (PM) probe and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)

> **Tip** You can use the `PMIntensities` matrix returned by the `celintensityread` function.

MMMatrix
: Matrix of intensity values where each row corresponds to a mismatch (MM) probe and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)

> **Tip** You can use the `MMIntensities` matrix returned by the `celintensityread` function.

AffinPM
: Column vector of PM probe affinities, such as returned by the `affyprobeaffinities` function. Each row corresponds to a probe.

AffinMM
: Column vector of MM probe affinities, such as returned by the `affyprobeaffinities` function. Each row corresponds to a probe.

OpticalCorrValue
: Controls the use of optical background correction on the PM and MM probe intensity values in *PMMatrix* and *MMMatrix*. Choices are `true` (default) or `false`.

CorrConstValue	Value that specifies the correlation constant, rho, for log background intensity for each PM/MM probe pair. Choices are any value ≥ `0` and ≤ `1`. Default is `0.7`.
MethodValue	String that specifies the method to estimate the signal. Choices are `MLE`, a faster, ad hoc Maximum Likelihood Estimate method, or `EB`, a slower, more formal, empirical Bayes method. Default is `MLE`.
TuningParamValue	Value that specifies the tuning parameter used by the estimate method. This tuning parameter sets the lower bound of signal values with positive probability. Choices are a positive value. Default is `5` (MLE) or `0.5` (EB). **Tip** For information on determining a setting for this parameter, see Wu et al., 2004.
AddVarianceValue	Controls whether the signal variance is added to the weight function for smoothing low signal edge. Choices are `true` or `false` (default).

ShowplotValue	Controls the display of a plot showing the $\log_2$ of probe intensity values from a specified column (chip) in *MMMatrix*, versus probe affinities in *AffinMM*. Choices are `true`, `false`, or *I*, an integer specifying a column in *MMMatrix*. If set to `true`, the first column in *MMMatrix* is plotted. Default is: • `false` — When return values are specified. • `true` — When return values are not specified.
VerboseValue	Controls the display of a progress report showing the number of each chip as it is completed. Choices are `true` (default) or `false`.

Return Values

PMMatrix_Adj	Matrix of background adjusted PM (perfect match) intensity values.
nsbStruct	Structure containing nonspecific binding background parameters, estimated from the intensities and affinities of probes on an Affymetrix GeneChip array. *nsbStruct* includes the following fields: • `sigma` • `mu_pm` • `mu_mm`

Description

PMMatrix_Adj = gcrmabackadj(*PMMatrix*, *MMMatrix*, *AffinPM*, *AffinMM*) performs GCRMA background adjustment (including optical background correction and nonspecific binding correction) on Affymetrix microarray probe-level data, using probe sequence information and returns *PMMatrix_Adj*, a matrix of background adjusted PM (perfect match) intensity values.

Note If *AffinPM* and *AffinMM* data are not available, you can still use the gcrmabackadj function by entering empty column vectors for both of these inputs in the syntax.

[*PMMatrix_Adj*, *nsbStruct*] = gcrmabackadj(*PMMatrix*, *MMMatrix*, *AffinPM*, *AffinMM*) returns *nsbStruct*, a structure containing nonspecific binding background parameters, estimated from the intensities and affinities of probes on an Affymetrix GeneChip array. *nsbStruct* includes the following fields:

- sigma
- mu_pm
- mu_mm

... = gcrmabackadj(...'*PropertyName*', *PropertyValue*, ...) calls gcrmabackadj with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

... = gcrmabackadj(...'OpticalCorr', *OpticalCorrValue*, ...) controls the use of optical background correction on the PM and MM probe intensity values in *PMMatrix* and *MMMatrix*. Choices are true (default) or false.

... = gcrmabackadj(...'CorrConst', *CorrConstValue*, ...) specifies the correlation constant, rho, for log background intensity for each PM/MM probe pair. Choices are any value ≥ 0 and ≤ 1. Default is 0.7.

... = gcrmabackadj(...'Method', *MethodValue*, ...) specifies the method to estimate the signal. Choices are MLE, a faster, ad hoc Maximum Likelihood Estimate method, or EB, a slower, more formal, empirical Bayes method. Default is MLE.

`... = gcrmabackadj( ...'TuningParam', TuningParamValue, ...)` specifies the tuning parameter used by the estimate method. This tuning parameter sets the lower bound of signal values with positive probability. Choices are a positive value. Default is `5` (MLE) or `0.5` (EB).

Tip For information on determining a setting for this parameter, see Wu et al., 2004.

`... = gcrmabackadj( ...'AddVariance', AddVarianceValue, ...)` controls whether the signal variance is added to the weight function for smoothing low signal edge. Choices are `true` or `false` (default).

`... = gcrmabackadj( ...'Showplot', ShowplotValue, ...)` controls the display of a plot showing the $\log_2$ of probe intensity values from a specified column (chip) in *`MMMatrix`*, versus probe affinities in *`AffinMM`*. Choices are `true`, `false`, or *`I`*, an integer specifying a column in *`MMMatrix`*. If set to `true`, the first column in *`MMMatrix`* is plotted. Default is:

- `false` — When return values are specified.
- `true` — When return values are not specified.

`... = gcrmabackadj( ...'Verbose', VerboseValue, ...)` controls the display of a progress report showing the number of each chip as it is completed. Choices are `true` (default) or `false`.

Examples

1. Load the MAT file, included with Bioinformatics Toolbox, that contains Affymetrix data from a prostate cancer study. The variables in the MAT file include `seqMatrix`, a matrix containing sequence information for PM probes, `pmMatrix` and `mmMatrix`, matrices containing PM and MM probe intensity values, and `probeIndices`, a column vector containing probe indexing information.

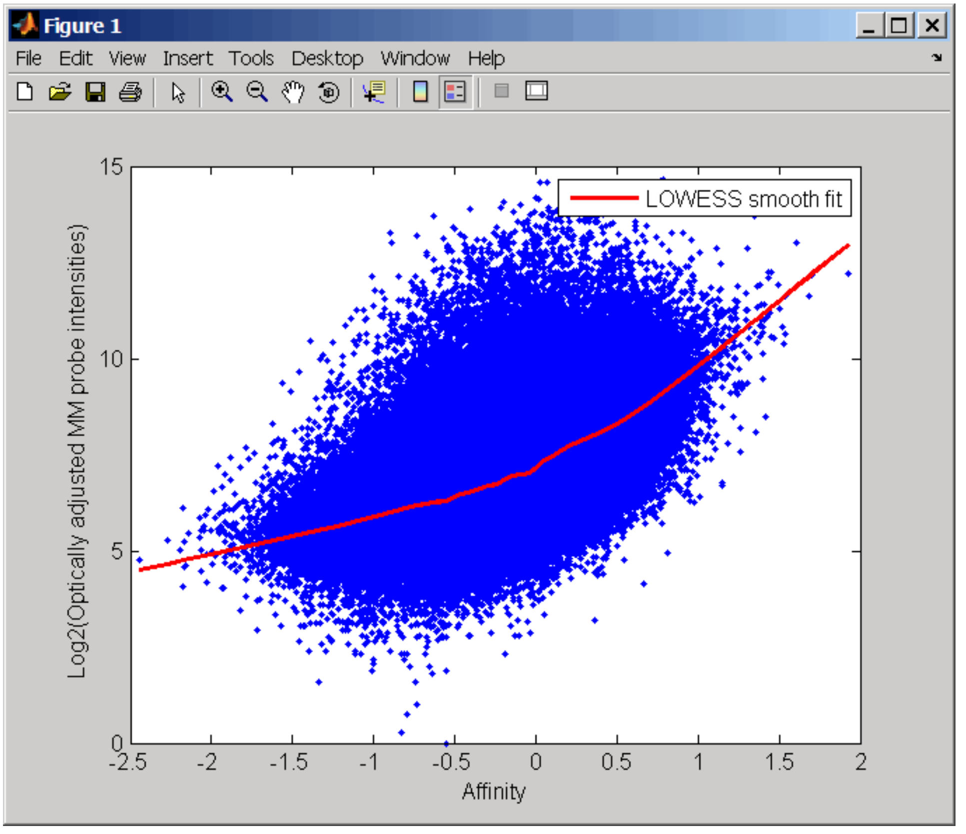
   ```
   load prostatecancerrawdata
   ```

2 Compute the Affymetrix PM and MM probe affinities from their sequences and MM probe intensities.

```
[apm, amm] = affyprobeaffinities(seqMatrix, mmMatrix(:,1),...
             'ProbeIndices', probeIndices);
```

3 Perform GCRMA background adjustment on the Affymetrix microarray probe-level data, creating a matrix of background adjusted PM intensity values. Also, display a plot showing the $\log_2$ of probe intensity values from column 3 (chip 3) in `mmMatrix`, versus probe affinities in `amm`.

```
pms_adj = gcrmabackadj(pmMatrix, mmMatrix, apm, amm, 'showplot', 3);
```



4 Perform GCRMA background adjustment again, using the slower, more formal, empirical Bayes method.

```
pms_adj2 = gcrmabackadj(pmMatrix, mmMatrix, apm, amm, 'method', 'EB');
```

The `prostatecancerrawdata.mat` file used in this example contains data from Best et al., 2005.

References

[1] Wu, Z., Irizarry, R.A., Gentleman, R., Murillo, F.M., and Spencer, F. (2004). A Model Based Background Adjustment for Oligonucleotide

Expression Arrays. Journal of the American Statistical Association *99(468)*, 909–917.

[2] Wu, Z., and Irizarry, R.A. (2005). Stochastic Models Inspired by Hybridization Theory for Short Oligonucleotide Arrays. Proceedings of RECOMB 2004. J Comput Biol. *12(6)*, 882–93.

[3] Wu, Z., and Irizarry, R.A. (2005). A Statistical Framework for the Analysis of Microarray Probe-Level Data. Johns Hopkins University, Biostatistics Working Papers 73.

[4] Wu, Z., and Irizarry, R.A. (2003). A Model Based Background Adjustment for Oligonucleotide Expression Arrays. RSS Workshop on Gene Expression, Wye, England, `http://biosun01.biostat.jhsph.edu/%7Ririzarr/Talks/gctalk.pdf`.

[5] Abd Rabbo, N.A., and Barakat, H.M. (1979). Estimation Problems in Bivariate Lognormal Distribution. Indian J. Pure Appl. Math *10(7)*, 815–825.

[6] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

See Also

Bioinformatics Toolbox functions: `affyprobeseqread`, `affyread`, `celintensityread`, `probelibraryinfo`

Purpose

Read data from GenBank file

Syntax

GenBankData = genbankread(*File*)

Arguments

File	Either of the following: • String specifying a file name, a path and file name, or a URL pointing to a file. The referenced file is a GenBank-formatted file (ASCII text file). If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Directory. • MATLAB character array that contains the text of a GenBank-formatted file.
GenBankData	MATLAB structure with fields corresponding to GenBank keywords.

Description

GenBankData = genbankread(*File*) reads in a GenBank-formatted file, *File*, and creates a structure, *GenBankData*, containing fields corresponding to the GenBank keywords. Each separate sequence listed in the output structure *GenBankData* is stored as a separate element of the structure.

Examples

1. Get sequence information for a gene (HEXA), store data in a file, and then read back into MATLAB.

```
getgenbank('nm_000520', 'ToFile', 'TaySachs_Gene.txt')
s = genbankread('TaySachs_Gene.txt')

s =

                LocusName: 'NM_000520'
      LocusSequenceLength: '2255'
     LocusNumberofStrands: ''
```

```
              LocusTopology: 'linear'
          LocusMoleculeType: 'mRNA'
       LocusGenBankDivision: 'PRI'
      LocusModificationDate: '13-AUG-2006'
                 Definition: [1x63 char]
                  Accession: 'NM_000520'
                    Version: 'NM_000520.2'
                         GI: '13128865'
                    Project: []
                   Keywords: []
                    Segment: []
                     Source: 'Homo sapiens (human)'
             SourceOrganism: [4x65 char]
                  Reference: {1x58 cell}
                    Comment: [15x67 char]
                   Features: [74x74 char]
                        CDS: [1x1 struct]
                   Sequence: [1x2255 char]
```

2 Display the source organism for this sequence.

```
s.SourceOrganism

ans =

Homo sapiens
Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;
Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini;
Catarrhini; Hominidae; Homo.
```

See Also

Bioinformatics Toolbox functions: `emblread`, `fastaread`, `genpeptread`, `getgenbank`, `scfread`, `seqtool`

Purpose

Remove genes with low entropy expression values

Syntax

```
Mask = geneentropyfilter(Data)
[Masks, FData] = geneentropyfilter(Data)
[Mask, FData, FNames] = geneentropyfilter(Data,Names)
geneentropyfilter(..., 'PropertyName', PropertyValue,...)
geneentropyfilter(..., 'Percentile', PercentileValue)
```

Arguments

Data	Matrix where each row corresponds to the experimental results for one gene. Each column is the results for all genes from one experiment.
Names	Cell array with the name of a gene for each row of experimental data. *Names* has same number of rows as *Data* with each row containing the name or ID of the gene in the data set.
PercentileValue	Property to specify a percentile below which gene data is removed. Enter a value from 0 to 100.

Description

Mask = geneentropyfilter(*Data*) identifies gene expression profiles in *Data* with entropy values less than the 10th percentile.

Mask is a logical vector with one element for each row in Data. The elements of *Mask* corresponding to rows with a variance greater than the threshold have a value of 1, and those with a variance less then the threshold are 0.

[*Masks, FData*] = geneentropyfilter(*Data*) returns a filtered data matrix (*FData*). *FData* can also be created using *FData* = Data(find(I),:).

[*Mask, FData, FNames*] = geneentropyfilter(*Data,Names*) returns a filtered names array (*FNames*). You can also create *FNames* using *FNames* = Names(I).

geneentropyfilter(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

`geneentropyfilter(..., 'Percentile', PercentileValue)` removes from the experimental data (*Data*) gene expression profiles with entropy values less than a given percentile (*PercentileValue*).

Examples

```
load yeastdata
[fyeastvalues, fgenes] = geneentropyfilter(yeastvalues,genes);
```

References

[1] Kohane I.S., Kho A.T., Butte A.J. (2003), Microarrays for an Integrative Genomics, Cambridge, MA:MIT Press.

See Also

Bioinformatics Toolbox functions: `exprprofrange`, `exprprofvar`, `genelowvalfilter`, `generangefilter`, `genevarfilter`

Purpose Remove gene profiles with low absolute values

Syntax

```
Mask = genelowvalfilter(Data)
[Mask, FData] = genelowvalfilter(Data)
[Mask, FData, FNames] = genelowvalfilter(Data, Names)
genelowvalfilter(..., 'PropertyName', PropertyValue,...)
genelowvalfilter(..., 'Prctile', PrctileValue)
genelowvalfilter(..., 'AbsValue', AbsValueValue)
genelowvalfilter(..., 'AnyVal', AnyValValue)
```

Arguments

Data	Matrix where each row corresponds to the experimental results for one gene. Each column is the results for all genes from one experiment.
Names	Cell array with the same number of rows as *Data*. Each row contains the name or ID of the gene in the data set.
PrctileValue	Property to specify a percentile below which gene expression profiles are removed. Enter a value from 0 to 100.
AbsValueValue	Property to specify an absolute value below which gene expression profiles are removed.
AnyValValue	Property to select the minimum or maximum absolute value for comparison with *AbsValueValue*. If *AnyValValue* is true, selects the minimum absolute value. If *AnyValValue* is false, selects the maximum absolute value. The default value is false.

Description Gene expression profile experiments have data where the absolute values are very low. The quality of this type of data is often bad due to large quantization errors or simply poor spot hybridization.

Mask = genelowvalfilter(*Data*) identifies gene expression profiles in Data with all absolute values less than the 10th percentile.

Mask is a logical vector with one element for each row in *Data*. The elements of *Mask* corresponding to rows with absolute expression levels greater than the threshold have a value of 1, and those with absolute expression levels less then the threshold are 0.

[*Mask*, *FData*] = genelowvalfilter(*Data*) returns a filtered data matrix (*FData*). You can create *FData* using *FData* = Data(find(*I*),:).

[*Mask, FData, FNames*] = genelowvalfilter(*Data*, *Names*) returns a filtered names array (*FNames*), where *Names* is a cell array of the names of the genes corresponding to each row of *Data*. You can also create *FNames* using *FNames* = Names(I).

genelowvalfilter(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

genelowvalfilter(..., 'Prctile', *PrctileValue*) removes from the experimental data (*Data*) gene expression profiles with all absolute values less than a specified percentile (*Percentile*).

genelowvalfilter(..., 'AbsValue', *AbsValueValue*) calculates the maximum absolute value for each gene expression profile and removes the profiles with maximum absolute values less than *AbsValValue*.

genelowvalfilter(..., 'AnyVal', *AnyValValue*), when *AnyValValue* is true, calculates the minimum absolute value for each gene expression profile and removes the profiles with minimum absolute values less than *AnyValValue*.

Examples

```
[data, labels, I, FI] = genelowvalfilter(data,labels,'AbsValue',5);
```

References

[1] Kohane I.S., Kho A.T., Butte A.J. (2003), Microarrays for an Integrative Genomics, Cambridge, MA:MIT Press.

See Also

Bioinformatics Toolbox functions: exprprofrange, exprprofvar, geneentropyfilter, generangefilter, genevarfilter

Purpose Create `geneont object`

Syntax

```
GeneontObj = geneont
GeneontObj = geneont('File', FileValue)
GeneontObj = geneont('Live', LiveValue)
GeneontObj = geneont('Live', LiveValue,
'ToFile', ToFileValue)
```

Arguments

FileValue	file name of an OBO-formatted file that is on the MATLAB search path.
LiveValue	Property to create the most up-to-date geneont object. Enter `true` to create a geneont object (*GeneontObj*) from the most recent version of the Gene Ontology database. Default is `false`.
ToFileValue	file name to which to save the geneont object from the Gene Ontology database.

Description

GeneontObj `= geneont` searches for the file `gene_ontology.obo` in the MATLAB Current Directory and creates a geneont object.

GeneontObj `= geneont('File',` *FileValue*`)` creates a geneont object (*GeneontObj*) from an OBO-formatted file that is on the MATLAB search path.

GeneontObj `= geneont('Live',` *LiveValue*`)`, when *LiveValue* is `true`, creates a geneont object (*GeneontObj*) from the most recent version of the Gene Ontology database, which is the file at

```
http://www.geneontology.org/ontology/gene_ontology.obo
```

Note The full Gene Ontology database may take several minutes to download when you run this function using the Live property.

GeneontObj = geneont('Live', *LiveValue*, 'ToFile', *ToFileValue*), when *LiveValue* is true, creates a geneont object (*GeneontObj*) from the file at

```
http://www.geneontology.org/ontology/gene_ontology.obo
```

and saves the file to a local file ('*ToFileValue*').

Examples

1 Download the Gene Ontology database from the Web into MATLAB.

```
GO = geneont('LIVE', true);
```

MATLAB creates a geneont object and displays the number of terms in the database.

```
Gene Ontology object with 20005 Terms.
```

2 Display information about the geneont object.

```
get(GO)

default_namespace: 'gene_ontology'
   format_version: '1.0'
             date: '01:11:2005 16:51'
            Terms: [20005x1 geneont.term]
```

3 Search for all GO terms in the geneont object that contain the string ribosome in the property field name and create a structure of those terms.

```
comparison = regexpi(get(GO.Terms,'name'),'ribosome');
indices = find(~cellfun('isempty',comparison));
terms_with_ribosmome = GO.Term(indices)
23x1 struct array with fields:
    id
    name
    ontology
    definition
    synonym
```

```
is_a
part_of
obsolete
```

See Also

Bioinformatics Toolbox functions: `goannotread`, `num2goid`

Bioinformatics Toolbox object: `geneont object`

Bioinformatics Toolbox methods of geneont object: `getancestors`, `getdescendants`, `getmatrix`, `getrelatives`

generangefilter

Purpose

Remove gene profiles with small profile ranges

Syntax

```
Mask = generangefilter(Data)
[Mask, FData] = generangefilter(Data)
[Mask, FData, FNames] = generangefilter(Data,Names)
generangefilter(..., 'PropertyName', PropertyValue,...)
generangefilter(..., 'Percentile', PercentileValue)
generangefilter(..., 'AbsValue', AbsValueValue)
generangefilter(..., 'LOGPercentile', LOGPercentileValue)
generangefilter(..., 'LOGValue', LOGValueValue)
```

Arguments

Data	Matrix where each row corresponds to the experimental results for one gene. Each column is the results for all genes from one experiment.
Names	Cell array with the name of a gene for each row of experimental data. *Names* has same number of rows as *Data* with each row containing the name or ID of the gene in the data set.
PercentileValue	Property to specify a percentile below which gene expression profiles are removed. Enter a value from `0` to `100`.
AbsValueValue	Property to specify an absolute value below which gene expression profiles are removed.
LOGPercentileValue	Property to specify the LOG of a percentile.
LOGValueValue	Property to specify the LOG of an absolute value.

Description

Mask = `generangefilter(`*Data*`)` calculates the range for each gene expression profile in the experimental data (*Data*), and then identifies the expression profiles with ranges less than the `10`th percentile.

Mask is a logical vector with one element for each row in *Data*. The elements of *Mask* corresponding to rows with a range greater then the threshold have a value of 1, and those with a range less then the threshold are 0.

[*Mask, FData*] = generangefilter(*Data*) returns a filtered data matrix (*FData*). *FData* can also be created using *FData* = Data(find(I),:).

[*Mask, FData, FNames*] = generangefilter(*Data,Names*) returns a filtered names array (*FNames*), where *Names* is a cell array with the names of the genes corresponding to each row in *Data*. You can also create *FNames* using *FNames* = Names(I).

generangefilter(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

generangefilter(..., 'Percentile', *PercentileValue*) removes from the experimental data (*Data*) gene expression profiles with ranges less than a specified percentile (*PercentileValue*).

generangefilter(..., 'AbsValue', *AbsValueValue*) removes from *Data* gene expression profiles with ranges less than *AbsValueValue*.

generangefilter(..., 'LOGPercentile', *LOGPercentileValue*) filters genes with profile ranges in the lowest percent of the log range (*LOGPercentileValue*).

generangefilter(..., 'LOGValue', *LOGValueValue*) filters genes with profile log ranges lower than *LOGValueValue*.

Examples

```
load yeastdata
[mask, fyeastvalues, fgenes] = generangefilter(yeastvalues,genes);
```

References

[1] Kohane I.S., Kho A.T., Butte A.J. (2003), Microarrays for an Integrative Genomics, Cambridge, MA:MIT Press.

See Also

Bioinformatics Toolbox functions: exprprofrange, exprprofvar, geneentropyfilter, genelowvalfilter, genevarfilter

geneticcode

Purpose

Nucleotide codon to amino acid mapping

Syntax

```
Map = geneticcode
geneticcode(GeneticCode)
```

Arguments

GeneticCode	Enter a code number or code name from the table . If you use a code name, you can truncate the name to the first two characters of the name.

Genetic Code

Code Number	Code Name
1	Standard
2	Vertebrate Mitochondrial
3	Yeast Mitochondrial
4	Mold, Protozoan, Coelenterate Mitochondrial, and Mycoplasma/Spiroplasma
5	Invertebrate Mitochondrial
6	Ciliate, Dasycladacean, and Hexamita Nuclear
9	Echinoderm Mitochondrial
10	Euplotid Nuclear
11	Bacterial and Plant Plastid
12	Alternative Yeast Nuclear
13	Ascidian Mitochondrial
14	Flatworm Mitochondrial
15	Blepharisma Nuclear
16	Chlorophycean Mitochondrial

Code Number	Code Name
21	Trematode Mitochondrial
22	Scenedesmus Obliquus Mitochondrial
23	Thraustochytrium Mitochondrial

Description

Map = geneticcode returns a structure with a mapping of nucleotide codons to amino acids for the standard genetic code.

geneticcode(*GeneticCode*) returns a structure of the mapping for alternate genetic codes, where *GeneticCode* is either of the following:

- The transl_table (code) number from the NCBI Genetics Web page

  http://www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=c

- One of the supported names in the table above

Examples

List the mapping of nucleotide codons to amino acids for a specific genetic code.

```
wormcode = geneticcode('Flatworm Mitochondrial');
```

See Also

Bioinformatics Toolbox functions: aa2nt, aminolookup, baselookup, codonbias, dnds, dndsml, nt2aa, revgeneticcode, seqshoworfs, seqtool

genevarfilter

Purpose

Filter genes with small profile variance

Syntax

```
Mask = genevarfilter(Data)
[Mask, FData] = genevarfilter(Data)
[Mask, FData, FNames] = genevarfilter(Data,Names)
genevarfilter(..., 'PropertyName', PropertyValue,...)
genevarfilter(..., 'Percentile', PercentileValue)
genevarfilter(..., 'AbsValue', AbsValValue)
```

Arguments

Data	Matrix where each row corresponds to a gene. The first column is the names of the genes, and each additional column is the results from an experiment.
Names	Cell array with the name of a gene for each row of experimental data. *Names* has same number of rows as *Data* with each row containing the name or ID of the gene in the data set.
Percentile	Property to specify a percentile below which gene expression profiles are removed. Enter a value from `0` to `100`.
AbsValue	Property to specify an absolute value below which gene expression profiles are removed.

Description

Gene profiling experiments have genes that exhibit little variation in the profile and are generally not of interest in the experiment. These genes are commonly removed from the data.

`Mask = genevarfilter(Data)` calculates the variance for each gene expression profile in `Data` and then identifies the expression profiles with a variance less than the `10`th percentile.

`Mask` is a logical vector with one element for each row in *Data*. The elements of `Mask` corresponding to rows with a variance greater than the threshold have a value of `1`, and those with a variance less than the threshold are `0`.

`[Mask, FData] = genevarfilter(Data)` returns the filtered data matrix (`FData`). You can also create `FData` using `FData = Data(find(I),:)`.

`[Mask, FData, FNames] = genevarfilter(Data,Names)` returns a filtered names array (`FNames`). `Names` is a cell array of the names of the genes corresponding to each row of Data. `FNames` can also be created using `FNames = Names(I)`.

`genevarfilter(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`genevarfilter(..., 'Percentile', PercentileValue)` removes from the experimental data (`Data`) gene expression profiles with a variance less than the percentile (`Percentile`).

`genevarfilter(..., 'AbsValue', AbsValValue)` removes from `Data` gene expression profiles with a variance less than `AbsValue`.

Examples

```
load yeastdata
[fyeastvalues, fgenes] = genevarfilter(yeastvalues,genes);
```

References

[1] Kohane I.S., Kho A.T., Butte A.J. (2003), Microarrays for an Integrative Genomics, Cambridge, MA:MIT Press.

See Also

Bioinformatics Toolbox functions: `exprprofrange`, `exprprofvar`, `generangefilter`, `geneentropyfilter`, `genelowvalfilter`

genpeptread

Purpose

Read data from GenPept file

Syntax

```
GenPeptData = genpeptread('File')
```

Arguments

File	GenPept formatted file (ASCII text file). Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text of a GenPept file.

Description

`genpeptread` reads data from a GenPept formatted file into a MATLAB structure.

Note NCBI has changed the name of their protein search engine from GenPept to Entrez Protein. However, the function names in Bioinformatics Toolbox (`getgenpept` and `genpeptread`) are unchanged representing the still-used GenPept report format.

`GenPeptData = genpeptread('File')` reads in the GenPept formatted sequence from *File* and creates a structure `GenPeptData`, containing fields corresponding to the GenPept keywords. Each separate sequence listed in *File* is stored as a separate element of the structure. `GenPeptDATA` contains these fields:

Field
LocusName
LocusSequenceLength
LocusMoleculeType
LocusGenBankDivision
LocusModificationDate
Definition

Field
Accession
PID
Version
GI
DBSource
Keywords
Source
SourceDatabase
SourceOrganism
Reference.Number
Reference.Authors
Reference.Title
Reference.Journal
Reference.MedLine
Reference.PubMed
Reference.Remark
Comment
Features
Weight
Length
Sequence

Examples

Get sequence information for the protein coded by the gene HEXA, save to a file, and then read back into MATLAB.

```
getgenpept('p06865', 'ToFile', 'TaySachs_Protein.txt')
genpeptread('TaySachs_Protein.txt')
```

See Also

Bioinformatics Toolbox functions: `fastaread`, `genbankread`, `getgenpept`, `pdbread`, `seqtool`

Purpose Read Gene Expression Omnibus (GEO) SOFT format data

Syntax

```
GEOSOFTData = geosoftread(File)
```

Arguments

File	Gene Expression Omnibus (GEO) SOFT format Sample file (GSM) or Data Set file (GDS). Enter a file name, a path and file name, or a URL pointing to a file.

Note *File* can also be a MATLAB character array that contains the text of a GEO file.

Description

GEOSOFTData = geosoftread(*File*) reads a Gene Expression Omnibus (GEO) SOFT format Sample file (GSM) or Data Set file (GDS), and then creates a MATLAB structure, *GEOSOFTdata*, with the following fields.

Fields
Scope
Accession
Header
ColumnDescriptions
ColumnNames
Data
Identifier (GDS files only)
IDRef (GDS files only)

Fields correspond to the GenBank keywords. Each separate entry listed in *File* is stored as a separate element of the structure.

Examples

Get data from the GEO Web site and save it to a file.

```
geodata = getgeodata('GSM3258','ToFile','GSM3258.txt');
```

Use `geosoftread` to access a local copy of a GEO file instead of accessing it from the GEO Web site.

```
geodata = geosoftread('GSM3258.txt')
```

See Also

Bioinformatics Toolbox functions: `galread`, `getgeodata`, `gprread`, `sptread`

Purpose

BLAST report from NCBI Web site

Syntax

```
Data = getblast(RID)
getblast(..., 'PropertyName', PropertyValue,...)
getblast(..., 'Descriptions', DescriptionsValue)
getblast(..., 'Alignments', AlignmentsValue)
getblast(..., 'ToFile', ToFileValue)
getblast(..., 'FileFormat', FileFormatValue)
getblast(..., 'WaitTime', WaitTimeValue)
```

Arguments

RID	BLAST Request ID (*RID*) from the function `blastncbi`.
DescriptionsValue	Property to specify the number of descriptions in a report.
AlignmentsValue	Property to select the number of alignments in a report. Enter values from `1` to `100`. The default value is `50`.
ToFileValue	Property to specify a file name for saving report data.
FileFormatValue	Property to select the format of the file named in `ToFileValue`. Enter either `'TEXT'` or `'HTML'`. Default is `'TEXT'`.
WaitTimeValue	Property to pause MATLAB and wait a specified time (minutes) for a report from the NCBI Web site. If the report is still not available after the wait time, `getblast` returns an error message. The default behavior is to not wait for a report.

Description

BLAST (Basic Local Alignment Search Tool) reports offer a fast and powerful comparative analysis of interesting protein and nucleotide sequences against known structures in existing online databases. `getblast` parses NCBI BLAST reports, including `BLASTN`, `BLASTP`, `BLASTX`, `TBLASTN`, `TBLASTX`, and `psi-BLAST`.

`Data = getblast(RID)` reads a BLAST Request ID (`RID`) and returns the report data in a structure (`Data`). The NCBI Request ID (`RID`) must be a recently generated report because NCBI purges reports after 24 hours.

`getblast(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`getblast(..., 'Descriptions', DescriptionsValue)` includes the specified number of descriptions (`DescriptionsValue`) in the report.

`getblast(..., 'Alignments', AlignmentsValue)` includes the specified number of alignments in the report.

`getblast(..., 'ToFile', ToFileValue)` saves the data returned from the NCBI BLAST report to a file (`ToFileValue`). The default format for the file is text, but you can specify HTML with the property `FileFormat`.

`getblast(..., 'FileFormat', FileFormatValue)` returns the report in the specified format (`FileFormatValue`).

`getblast(..., 'WaitTime', WaitTimeValue)` pauses MATLAB and waits a specified time (minutes) for a report from the NCBI Web site. If the report is still unavailable after the wait time, `getblast` returns an error message. The default behavior is to not wait for a report.

For more information about reading and interpreting BLAST reports, see:

```
http://www.ncbi.nlm.nih.gov/Education/BLASTinfo/tut1.html
```

Examples

1 Run a BLAST search with an NCBI accession number.

```
RID = blastncbi('AAA59174','blastp','expect',1e-10)
```

2 Pass the RID to GETBLAST to parse the report, load it into a MATLAB structure, and save a copy as a text file.

```
report = getblast(RID,'TOFILE','Report.txt')
```

See Also

Bioinformatics Toolbox functions: `blastncbi`, `blastread`

getembl

Purpose Sequence information from EMBL database

Syntax

```
Data = getembl('AccessionNumber)
getembl(..., 'PropertyName', PropertyValue,...)
getembl(..., 'ToFile', ToFileValue)
getembl(..., 'SequenceOnly', SequenceOnlyValue)
```

Arguments

AccessionNumber	Unique identifier for a sequence record. Enter a unique combination of letters and numbers.
ToFileValue	Property to specify the location and file name for saving data. Enter either a file name or a path and file name supported by your system (ASCII text file).
SequenceOnlyValue	Property to control getting a sequence without the metadata. Enter either `true` or `false` (default).

Description

`getembl` retrieves information from the European Molecular Biology Laboratory (EMBL) database for nucleotide sequences. This database is maintained by the European Bioinformatics Institute (EBI). For more details about the EMBL-Bank database, see

`http://www.ebi.ac.uk/embl/Documentation/index.html`

Data = `getembl('`*AccessionNumber*`)` searches for the accession number in the EMBL database (`http://www.ebi.ac.uk/embl`) and returns a MATLAB structure containing the following fields:

Field
`Comments`
`Identification`
`Accession`

Field
SequenceVersion
DateCreated
DateUpdated
Description
Keyword
OrganismSpecies
OrganismClassification
Organelle
Reference
DatabaseCrossReference
Feature
BaseCount
Sequence

`getembl(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`getembl(..., 'ToFile', ToFileValue)` returns a structure containing information about the sequence and saves the information in a file using an EMBL data format. If you do not give a location or path to the file, the file is stored in the MATLAB current directory. Read an EMBL formatted file back into MATLAB using the function `emblread`.

`getembl(..., 'SequenceOnly', SequenceOnlyValue)` , if *`SequenceOnlyValue`* is `true`, returns the sequence information without the metadata.

Examples

Retrieve data for the rat liver apolipoprotein A-I.

```
emblout = getembl('X00558')
```

Retrieve data for the rat liver apolipoprotein and save in the file rat_protein. If a file name is given without a path, the file is stored in the current directory.

```
Seq = getembl('X00558','ToFile','c:\project\rat_protein.txt')
```

Retrieve only the sequence for the rat liver apolipoprotein.

```
Seq = getembl('X00558','SequenceOnly',true)
```

See Also

Bioinformatics Toolbox functions: emblread, getgenbank, getgenpept, getpdb, seqtool

Purpose

Sequence information from GenBank database

Syntax

```
Data = getgenbank('AccessionNumber')
getgenbank('AccessionNumber')
getgenbank(..., 'PropertyName', PropertyValue,...)
getgenbank(..., 'ToFile', ToFileValue)
getgenbank(..., 'FileFormat', FileFormatValue)
getgenbank(..., 'SequenceOnly', SequenceOnlyValue)
```

Arguments

AccessionNumber	Unique identifier for a sequence record. Enter a unique combination of letters and numbers.
ToFileValue	Property to specify the location and file name for saving data. Enter either a file name or a path and file name supported by your system (ASCII text file).
FileFormatValue	Property to select the format for the file specified with the property ToFileValue. Enter either `'GenBank'` or `'FASTA'`.
SequenceOnlyValue	Property to control getting the sequence only. Enter either `true` or `false`.

Description

`getgenbank` retrieves nucleotide and amino acid sequence information from the GenBank database. This database is maintained by the National Center for Biotechnology Information (NCBI). For more details about the GenBank database, see

```
http://www.ncbi.nlm.nih.gov/Genbank/
```

`Data = getgenbank('AccessionNumber')` searches for the accession number in the GenBank database and returns a MATLAB structure containing information for the sequence. If an error occurs while retrieving the GenBank formatted information, then an attempt is make to retrieve the FASTA formatted data.

`getgenbank('AccessionNumber')` displays information in the MATLAB Command Window without returning data to a variable. The displayed information includes hyperlinks to the URLs for searching and retrieving data.

`getgenbank(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`getgenbank(..., 'ToFile', ToFileValue)` saves the data returned from GenBank in a file. If you do not give a location or path to the file, the file is stored in the MATLAB current directory. Read a GenBank formatted file back into MATLAB using the function `genbankread`.

`getgenbank(..., 'FileFormat', FileFormatValue)` returns the sequence in the specified format (*FileFormatValue*).

`getgenbank(..., 'SequenceOnly', SequenceOnlyValue)` when `SequenceOnly` is `true`, returns only the sequence as a character array. When the properties `SequenceOnly` and `ToFile` are used together, the output file is in the FASTA format.

Examples

To retrieve the sequence from chromosome 19 that codes for the human insulin receptor and store it in a structure, `S`, in the MATLAB Command Window, type:

```
S = getgenbank('M10051')

S =

                LocusName: 'HUMINSR'
      LocusSequenceLength: '4723'
     LocusNumberofStrands: ''
            LocusTopology: 'linear'
        LocusMoleculeType: 'mRNA'
     LocusGenBankDivision: 'PRI'
    LocusModificationDate: '06-JAN-1995'
               Definition: 'Human insulin receptor mRNA, complete cds.'
                Accession: 'M10051'
                  Version: 'M10051.1'
```

```
             GI: '186439'
        Project: []
       Keywords: 'insulin receptor; tyrosine kinase.'
        Segment: []
         Source: 'Homo sapiens (human)'
 SourceOrganism: [4x65 char]
      Reference: {[1x1 struct]}
        Comment: [14x67 char]
       Features: [51x74 char]
            CDS: [1x1 struct]
       Sequence: [1x4723 char]
      SearchURL: [1x105 char]
    RetrieveURL: [1x95 char]
```

See Also

Bioinformatics Toolbox functions: `genbankread`, `getembl`, `getgenpept`, `getpdb`,`seqtool`

getgenpept

Purpose

Retrieve sequence information from GenPept database

Syntax

```
Data = getgenpept('AccessionNumber')
getgenpept(...)
getgenpept(..., 'PropertyName', PropertyValue,...)
getgenpept(..., 'ToFile', ToFileValue)
getgenpept(..., 'FileFormat', FileFormatValue)
getgenpept(..., 'SequenceOnly', SequenceOnlyValue)
```

Arguments

AccessionNumber	Unique identifier for a sequence record. Enter a combination of letters and numbers.
ToFileValue	Property to specify the location and file name for saving data. Enter either a file name or a path and file name supported by your system (ASCII text file).
FileFormatValue	Property to select the format for the file specified with the property *ToFileValue*. Enter either `'GenBank'` or `'FASTA'`.
SequenceOnlyValue	Property to control getting the sequence without metadata. Enter either `true` or `false`.

Description

`getgenpept` retrieves a protein (amino acid) sequence and sequence information from the GenPept database. This database is a translation of the nucleotide sequences in GenBank and is maintained by the National Center for Biotechnology Information (NCBI).

Note NCBI has changed the name of their protein search engine from GenPept to Entrez Protein. However, the function names in Bioinformatics Toolbox (`getgenpept` and `genpeptread`) are unchanged representing the still-used GenPept report format.

For more details about the GenBank database, see

```
http://www.ncbi.nlm.nih.gov/Genbank/
```

Data = getgenpept('*AccessionNumber*') searches for the accession number in the GenPept database and returns a MATLAB structure containing for the sequence. If an error occurs while retrieving the GenBank formatted information, then an attempt is make to retrieve the FASTA formatted data.

getgenpept(...) displays the information to the screen without returning data to a variable. The displayed information includes hyperlinks to the URLs used to search for and retrieve the data.

getgenpept(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

getgenpept(..., 'ToFile', *ToFileValue*) saves the information in a file. If you do not give a location or path to the file, the file is stored in the MATLAB current directory. Read a GenPept formatted file back into MATLAB using the function genpeptread

getgenpept(..., 'FileFormat', *FileFormatValue*) returns the sequence in the specified format FileFormatValue.

getgenpept(..., 'SequenceOnly', *SequenceOnlyValue*) returns only the sequence information without the metadata if *SequenceOnlyValue* is true. When the properties SequenceOnly and ToFile are used together, the output file is in the FASTA format.

Examples

To retrieve the sequence for the human insulin receptor and store it in a structure, Seq, in the MATLAB Command Window, type:

```
Seq = getgenpept('AAA59174')

Seq =

                LocusName: 'AAA59174'
      LocusSequenceLength: '1382'
     LocusNumberofStrands: ''
```

```
           LocusTopology: 'linear'
       LocusMoleculeType: ''
    LocusGenBankDivision: 'PRI'
   LocusModificationDate: '06-JAN-1995'
              Definition: 'insulin receptor precursor.'
               Accession: 'AAA59174'
                 Version: 'AAA59174.1'
                      GI: '307070'
                 Project: []
                DBSource: 'locus HUMINSR accession M10051.1'
                Keywords: ''
                  Source: 'Homo sapiens (human)'
          SourceOrganism: [4x65 char]
               Reference: {[1x1 struct]}
                 Comment: [14x67 char]
                Features: [40x64 char]
                Sequence: [1x1382 char]
               SearchURL: [1x104 char]
             RetrieveURL: [1x92 char]
```

See Also

Bioinformatics Toolbox functions: genpeptread, getembl, getgenbank, getpdb

Purpose

Retrieve Gene Expression Omnibus (GEO) Sample (GSM) data

Syntax

```
Data = getgeodata('AccessionNumber')
getgeodata(..., 'PropertyName', PropertyValue,...)
getgeodata(..., 'ToFile', ToFileValue)
```

Arguments

AccessionNumber	Unique identifier for a sequence record. Enter a combination of letters and numbers.
ToFileValue	Property to specify the location and file name for saving data. Enter either a file name, or a path and file name supported by your system (ASCII text file).

Description

Data = getgeodata('*AccessionNumber*') searches for the accession number in the Gene Expression Omnibus database and returns a MATLAB structure containing the following fields:

Field
Scope
Accession
Header
ColumnDescriptions
ColumnNames
Data

getgeodata(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

getgeodata(..., 'ToFile', *ToFileValue*) saves the data returned from the database to a file. Read a GenPept formatted file back into MATLAB using the function gensoftread.

Note Currently, Bioinformatics Toolbox supports only Sample (GSM) records.

For more information, see

```
http://www.ncbi.nlm.nih.gov/About/disclaimer.html
```

Examples

```
geoStruct = getgeodata('GSM1768')
```

See Also

Bioinformatics Toolbox functions: `geosoftread`, `getgenbank`, `getgenpept`

Purpose

Retrieve multiple sequence alignment associated with hidden Markov model (HMM) profile from PFAM database

Syntax

```
AlignStruct = gethmmalignment(PFAMNumber)
AlignStruct = gethmmalignment(PFAMAccessNumber)
AlignStruct = gethmmalignment(..., 'ToFile',
ToFileValue, ...)
AlignStruct = gethmmalignment(..., 'Type', TypeValue, ...)
AlignStruct = gethmmalignment(..., 'Mirror', MirrorValue,
   ...)
AlignStruct = gethmmalignment(..., 'IgnoreGaps',
IgnoreGaps,
   ...)
```

Arguments

PFAMNumber	Integer specifying a protein family number of an HMM profile record in the PFAM database. For example, `2` is the protein family number for the protein family `PF0002`.
PFAMAccessNumber	String specifying a protein family accession number of an HMM profile record in the PFAM database. For example, `PF00002`.
ToFileValue	String specifying a file name or a path and file name for saving the data. If you specify only a file name, that file will be saved in the MATLAB Current Directory.
TypeValue	String that specifies the set of alignments returned. Choices are: • `full` — Default. Returns all alignments that fit the HMM profile. • `seed` — Returns only the alignments used to generate the HMM profile.

MirrorValue	String that specifies a Web database. Choices are: • `Sanger` (default) • `Janelia`
IgnoreGapsValue	Controls the removal of the symbols `-` and `.` from the sequence. Choices are `true` or `false` (default).

Return Values

AlignStruct	MATLAB structure containing the multiple sequence alignment associated with an HMM profile.

Description

AlignStruct = gethmmalignment(*PFAMNumber*) determines a protein family accession number from *PFAMNumber*, an integer, searches the PFAM database for the associated HMM profile record, retrieves the multiple sequence alignment associated with the HMM profile, and returns *AlignStruct*, a MATLAB structure containing the following fields:

Field
Header
Sequence

AlignStruct = gethmmalignment(*PFAMAccessNumber*) searches the PFAM database for the HMM profile record represented by *PFAMAccessNumber*, a protein family accession number, retrieves the multiple sequence alignment associated with the HMM profile, and returns *AlignStruct*, a MATLAB structure.

AlignStruct = gethmmalignment(..., '*PropertyName*', *PropertyValue*, ...) calls `gethmmalignment` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`AlignStruct = gethmmalignment(..., 'ToFile', ToFileValue, ...)` saves the data returned from the PFAM database to a file specified by *`ToFileValue`*.

Note You can read a FASTA-formatted file containing PFAM data back into MATLAB using the `fastaread` function.

`AlignStruct = gethmmalignment(..., 'Type', TypeValue, ...)` specifies the set of alignments returned. Choices are:

- `full` — Default. Returns all sequences that fit the HMM profile.
- `seed` — Returns only the sequences used to generate the HMM profile.

`AlignStruct = gethmmalignment(..., 'Mirror', MirrorValue, ...)` specifies a Web database. Choices are:

- `Sanger` (default)
- `Janelia`

You can reach other mirror sites by passing the complete URL to the `fastaread` function.

Note These mirror sites are maintained separately and may have slight variations.

For more information about the PFAM database, see:

```
http://www.sanger.ac.uk/Software/Pfam/
http://pfam.janelia.org/
```

AlignStruct = gethmmalignment(..., 'IgnoreGaps', *IgnoreGaps*, ...) controls the removal of the symbols - and . from the sequence. Choices are true or false (default).

Examples

To retrieve a multiple alignment of the sequences used to train the HMM profile for global alignment to the 7-transmembrane receptor protein in the secretin family, enter either of the following:

```
pfamalign = gethmmalignment(2,'Type','seed')

pfamalign = gethmmalignment('PF00002','Type','seed')

pfamalign =

32x1 struct array with fields:
    Header
    Sequence
```

See Also

Bioinformatics Toolbox functions: fastaread, gethmmprof, gethmmtree, multialignread, pfamhmmread

Purpose

Retrieve hidden Markov model (HMM) profile from PFAM database

Syntax

```
HMMStruct = gethmmprof(PFAMName)
HMMStruct = gethmmprof(PFAMNumber)
HMMStruct = gethmmprof(PFAMAccessNumber)
HMMStruct = gethmmprof(..., 'ToFile', ToFileValue, ...)
HMMStruct = gethmmprof(..., 'Mode', ModeValue, ...)
HMMStruct = gethmmprof(..., 'Mirror', MirrorValue, ...)
```

Arguments

PFAMName	String specifying a protein family name (unique identifier) of an HMM profile record in the PFAM database. For example, 7tm_2.
PFAMNumber	Integer specifying a protein family number of an HMM profile record in the PFAM database. For example, 2 is the protein family number for the protein family PF0002.
PFAMAccessNumber	String specifying a protein family accession number of an HMM profile record in the PFAM database. The string must include a version number appended at the end of the accession number. For example, PF00002.14.

Note While this is the most efficient way to query the PFAM database, version numbers can change, making your input invalid.

ToFileValue	String specifying a file name or a path and file name for saving the data. If you specify only a file name, that file will be saved in the MATLAB Current Directory.

ModeValue	String that specifies the returned alignment mode. Choices are: • `ls` — Default. Global alignment mode. • `fs` — Local alignment mode.
MirrorValue	String that specifies a Web database. Choices are: • `Sanger` (default) • `Janelia`

Return Values

HMMStruct	MATLAB structure containing information retrieved from the PFAM database.

Description

HMMStruct = gethmmprof(*PFAMName*) searches the PFAM database for the record represented by *PFAMName*, a protein family name, retrieves the HMM profile information, and stores it in *HMMStruct*, a MATLAB structure, with the following fields:

Field
`Name`
`PfamAccessionNumber`
`ModelDescription`
`ModelLength`
`Alphabet`
`MatchEmission`
`InsertEmission`
`NullEmission`
`BeginX`
`MatchX`

Field
`InsertX`
`DeleteX`
`FlankingInsertX`
`LoopX`
`NullX`

HMMStruct = gethmmprof(*PFAMNumber*) determines a protein family accession number from *PFAMNumber*, an integer, searches the PFAM database for the associated record, retrieves the HMM profile information, and stores it in *HMMStruct*, a MATLAB structure.

HMMStruct = gethmmprof(*PFAMAccessNumber*) searches the PFAM database for the record represented by *PFAMAccessNumber*, a protein family accession number, retrieves the HMM profile information, and stores it in *HMMStruct*, a MATLAB structure.

Note While this is the most efficient way to query the PFAM database, version numbers can change, making your input invalid.

HMMStruct = gethmmprof(..., '*PropertyName*', *PropertyValue*, ...) calls gethmmprof with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

HMMStruct = gethmmprof(..., 'ToFile', *ToFileValue*, ...) saves the data returned from the PFAM database in a file specified by *ToFileValue*.

Note You can read an HMM-formatted file back into MATLAB using the `pfamhmmread` function.

`HMMStruct = gethmmprof(..., 'Mode', ModeValue, ...)` specifies the returned alignment mode. Choices are:

- `ls` — Default. Global alignment mode.
- `fs` — Local alignment mode.

`HMMStruct = gethmmprof(..., 'Mirror', MirrorValue, ...)` specifies a Web database. Choices are:

- `Sanger` (default)
- `Janelia`

You can reach other mirror sites by passing the complete URL to the `pfamhmmread` function.

Note These mirror sites are maintained separately and may have slight variations.

For more information about the PFAM database, see:

```
http://www.sanger.ac.uk/Software/Pfam/
http://pfam.janelia.org/
```

Examples

To retrieve a hidden Markov model (HMM) profile for the global alignment of the 7-transmembrane receptor protein in the secretin family, enter either of the following:

```
hmm = gethmmprof(2)
```

```
hmm = gethmmprof('7tm_2')

hmm =

                    Name: '7tm_2'
     PfamAccessionNumber: 'PF00002.14'
        ModelDescription: [1x42 char]
             ModelLength: 296
                Alphabet: 'AA'
           MatchEmission: [296x20 double]
          InsertEmission: [296x20 double]
            NullEmission: [1x20 double]
                  BeginX: [297x1 double]
                  MatchX: [295x4 double]
                 InsertX: [295x2 double]
                 DeleteX: [295x2 double]
         FlankingInsertX: [2x2 double]
                   LoopX: [2x2 double]
                   NullX: [2x1 double]
```

See Also

Bioinformatics Toolbox functions: gethmmalignment, hmmprofalign, hmmprofstruct, pfamhmmread, showhmmprof

gethmmtree

Purpose

Phylogenetic tree data from PFAM database

Syntax

```
Tree = gethmmtree(AccessionNumber)
gethmmtree(..., 'PropertyName', PropertyValue,...)
gethmmtree(..., 'ToFile', ToFileValue)
gethmmtree(..., 'Type', TypeValue)
```

Arguments

AccessionNumber	Accession number in the PFAM database.
ToFileValue	Property to specify the location and file name for saving data. Enter either a file name or a path and file name supported by your system (ASCII text file).
TypeValue	Property to control which alignments are included in the tree. Enter either `'seed'` or `'full'` (default).

Description

`Tree = gethmmtree(AccessionNumber)` searches for the PFAM family accession number in the PFAM database and returns an object (`Tree`) containing a phylogenetic tree representative of the protein family.

`gethmmtree(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`gethmmtree(..., 'ToFile', ToFileValue)` saves the data returned from the PFAM database in the file *ToFileValue*.

`gethmmtree(..., 'Type', TypeValue)`, when *TypeValue* is `'seed'`, returns a tree with only the alignments used to generate the HMM model. When *TypeValue* is `'full'`, returns a tree with all of the alignments that match the model.

Examples

Retrieve a phylogenetic tree built from the multiple aligned sequences used to train the HMM profile model for global alignment. The PFAM accession number `PF00002` is for the 7-transmembrane receptor protein in the secretin family.

```
tree  = gethmmtree(2, 'type', 'seed')
tree  = gethmmtree('PF00002', 'type', 'seed')
```

See Also

Bioinformatics Toolbox functions: `gethmmalignment`, `phytreeread`

getpdb

Purpose

Retrieve protein structure data from Protein Data Bank (PDB) database

Syntax

```
PDBStruct = getpdb(PDBid)
PDBStruct = getpdb(PDBid,  ...'ToFile', ToFileValue, ...)
PDBStruct = getpdb(PDBid,  ...'SequenceOnly',
   SequenceOnlyValue, ...)
```

Arguments

PDBid

String specifying a unique identifier for a protein structure record in the PDB database.

Note Each structure in the PDB database is represented by a four-character alphanumeric identifier. For example, `4hhb` is the identifier for hemoglobin.

ToFileValue

String specifying a file name or a path and file name for saving the PDB-formatted data. If you specify only a file name, that file will be saved in the MATLAB Current Directory.

Tip After you save the protein structure record to a local PDB-formatted file, you can use the `pdbread` function to read the file into MATLAB offline or use the `molviewer` function to display and manipulate a 3-D image of the structure.

SequenceOnlyValue

Controls the return of the protein sequence only. Choices are `true` or `false` (default). If there is one sequence, it is returned as a character array. If there are multiple sequences, they are returned as a cell array.

Return Values

PDBStruct	MATLAB structure containing a field for each PDB record.

Description

The Protein Data Bank (PDB) database is an archive of experimentally determined 3-D biological macromolecular structure data. For more information about the PDB format, see:

```
http://www.rcsb.org/pdb/file_formats/pdb/pdbguide2.2/guide2.2_frame.html
```

`getpdb` retrieves protein structure data from the Protein Data Bank (PDB) database, which contains 3-D biological macromolecular structure data.

`*PDBStruct* = getpdb(*PDBid*)` searches the PDB database for the protein structure record specified by the identifier *PDBid* and returns the MATLAB structure *PDBStruct*, which contains a field for each PDB record. The following table summarizes the possible PDB records and the corresponding fields in the MATLAB structure *PDBStruct*:

PDB Database Record	Field in the MATLAB Structure
HEADER	Header
OBSLTE	Obsolete
TITLE	Title
CAVEAT	Caveat
COMPND	Compound
SOURCE	Source
KEYWDS	Keywords
EXPDTA	ExperimentData
AUTHOR	Authors
REVDAT	RevisionDate
SPRSDE	Superseded

PDB Database Record	Field in the MATLAB Structure
JRNL	Journal
REMARK 1	Remark1
REMARK *N* **Note** N equals 2 through 999.	Remark*n* **Note** n equals 2 through 999.
DBREF	DBReferences
SEQADV	SequenceConflicts
SEQRES	Sequence
FTNOTE	Footnote
MODRES	ModifiedResidues
HET	Heterogen
HETNAM	HeterogenName
HETSYN	HeterogenSynonym
FORMUL	Formula
HELIX	Helix
SHEET	Sheet
TURN	Turn
SSBOND	SSBond
LINK	Link
HYDBND	HydrogenBond
SLTBRG	SaltBridge
CISPEP	CISPeptides
SITE	Site

PDB Database Record	Field in the MATLAB Structure
CRYST1	Cryst1
ORIGXn	OriginX
SCALEn	Scale
MTRIXn	Matrix
TVECT	TranslationVector
MODEL	Model
ATOM	Atom
SIGATM	AtomSD
ANISOU	AnisotropicTemp
SIGUIJ	AnisotropicTempSD
TER	Terminal
HETATM	HeterogenAtom
CONECT	Connectivity

`PDBStruct = getpdb(PDBid, ...'PropertyName', PropertyValue, ...)` calls `getpdb` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`PDBStruct = getpdb(PDBid, ...'ToFile', ToFileValue, ...)` saves the data returned from the database to a PDB-formatted file, *ToFileValue*.

Tip After you save the protein structure record to a local PDB-formatted file, you can use the `pdbread` function to read the file into MATLAB offline or use the `molviewer` function to display and manipulate a 3-D image of the structure.

PDBStruct = getpdb(*PDBid*, ...'SequenceOnly', *SequenceOnlyValue*, ...) controls the return of the protein sequence only. Choices are true or false (default). If there is one sequence, it is returned as a character array. If there are multiple sequences, they are returned as a cell array.

The Sequence Field

The Sequence field is also a structure containing sequence information in the following subfields:

- NumOfResidues
- ChainID
- ResidueNames — Contains the three-letter codes for the sequence residues.
- Sequence — Contains the single-letter codes for the sequence residues.

Note If the sequence has modified residues, then the ResidueNames subfield might not correspond to the standard three-letter amino acid codes. In this case, the Sequence subfield will contain the modified residue code in the position corresponding to the modified residue. The modified residue code is provided in the ModifiedResidues field.

The Model Field

The Model field is also a structure or an array of structures containing coordinate information. If the MATLAB structure contains one model, the Model field is a structure containing coordinate information for that model. If the MATLAB structure contains multiple models, the Model field is an array of structures containing coordinate information for each model. The Model field contains the following subfields:

- Atom
- AtomSD

- AnisotropicTemp
- AnisotropicTempSD
- Terminal
- HeterogenAtom

The Atom Field

The Atom field is also an array of structures containing the following subfields:

- AtomSerNo
- AtomName
- altLoc
- resName
- chainID
- resSeq
- iCode
- X
- Y
- Z
- occupancy
- tempFactor
- segID
- element
- charge
- AtomNameStruct — Contains three subfields: chemSymbol, remoteInd, and branch.

Examples

Retrieve the structure information for the electron transport (heme) protein that has a PDB identifier of 5CYT, read the information into a MATLAB structure pdbstruct, and save the information to a PDB-formatted file electron_transport.pdb in the MATLAB Current Directory.

```
pdbstruct = getpdb('5CYT', 'ToFile', 'electron_transport.pdb')
```

See Also

Bioinformatics Toolbox functions: getembl, getgenbank, getgenpept, molviewer, pdbdistplot, pdbread, pdbwrite

Purpose

Annotations from Gene Ontology annotated file

Syntax

`Annotation = goannotread('File')`

Arguments

`File`

Description

`Annotation` = `goannotread('`*`File`*`')` converts the contents of a Gene Ontology annotated file (*`File`*) into an array of `structs` (*`Annotation`*). Files should have the structure specified in

```
http://www.geneontology.org/GO.annotation.shtml#file
```

A list with some annotated files can be found at

```
http://www.geneontology.org/GO.current.annotations.shtml
```

Examples

1. Open a Web browser to

   ```
   http://www.geneontology.org/GO.current.annotations.shtml
   ```

2. Download the file containing `GO` annotations for the gene products of *Saccharomyces cerevisiae* (`gene_association.sgd.gz`) to your MATLAB Current Directory.

3. Uncompress the file using the `gunzip` function.

   ```
   gunzip('gene_association.sgd.gz')
   ```

4. Read the file into MATLAB.

   ```
   SGDGenes = goannotread('gene_association.sgd');
   ```

5. Create a structure with `GO` annotations and get a list of genes.

   ```
   S = struct2cell(SGDGenes);
   genes = S(3,:)'
   ```

See Also

Bioinformatics Toolbox

- functions — `geneont` (object constructor), `num2goid`
- `geneont` object methods — `getancestors`, `getdescendants`, `getmatrix`, `getrelatives`

Purpose

Gonnet scoring matrix

Syntax

```
gonnet
```

Description

`gonnet` returns the Gonnet matrix.

The Gonnet matrix is the recommended mutation matrix for initially aligning protein sequences. Matrix elements are ten times the logarithmic of the probability that the residues are aligned divided by the probability that the residues are aligned by chance, and then matrix elements are normalized to 250 PAM units.

Expected score = `-0.6152`, Entropy = `1.6845` bits Lowest score = `-8`, Highest score = `14.2`

Order:

```
A R N D C Q E G H I L K M F P S T W Y V B Z X *
```

References

[1] Gaston H, Gonnet M, Cohen A, Benner S (1992), “Exhaustive matching of the entire protein sequence database”, Science, 256:1443-1445.

See Also

Bioinformatics Toolbox functions `blosum`, `dayhoff`, `pam`

Purpose

Read microarray data from GenePix Results (GPR) file

Syntax

```
GPRData = gprread('File')
gprread(..., 'PropertyName', PropertyValue,...)
gprread(..., 'CleanColNames', CleanColNamesValue)
```

Arguments

File	GenePix Results formatted file (file extension GPR). Enter a file name or a path and file name.
CleanColNamesValue	Property to control creating column names that MATLAB can use as variable names.

Description

`GPRData = gprread('File')` reads GenePix results data from *File* and creates a MATLAB structure (*GPRData*) with the following fields:

Field
Header
Data
Blocks
Columns
Rows
Names
IDs
ColumnNames
Indices
Shape

`gprread(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`gprread(..., 'CleanColNames', CleanColNamesValue)`. A `GPR` file may contain column names with spaces and some characters that MATLAB cannot use in MATLAB variable names. If *`CleanColNamesValue`* is `true`, `gprread` returns names in the field `ColumnNames` that are valid MATLAB variable names and names that you can use in functions. By default, *`CleanColNamesValue`* is `false` and the field `ColumnNames` may contain characters that are invalid for MATLAB variable names.

The field `Indices` of the structure contains MATLAB indices that can be used for plotting heat maps of the data.

For more details on the `GPR` format, see

```
http://www.moleculardevices.com/pages/software/gn_genepix_file_formats.html#gpr
```

```
http://www.moleculardevices.com/pages/software/gn_gpr_format_history.html
```

For a list of supported file format versions, see

```
http://www.moleculardevices.com/pages/software/gn_genepix_file_formats.html
```

GenePix is a registered trademark of Molecular Devices Corporation.

Examples

```
% Read in a sample GPR file and plot the median foreground
% intensity for the 635 nm channel.
gprStruct = gprread('mouse_a1pd.gpr')
maimage(gprStruct,'F635 Median');

% Alternatively you can create a similar plot using
% more basic graphics commands.
F635Median = magetfield(gprStruct,'F635 Median');
imagesc(F635Median(gprStruct.Indices));
colormap bone
colorbar;
```

See Also

Bioinformatics Toolbox functions: `affyread`, `agferead`, `celintensityread`, `galread`, `geosoftread`, `imageneread`, `magetfield`, `sptread`

Purpose

Find all shortest paths in graph

Syntax

```
[dist] = graphallshortestpaths(G)
[dist] = graphallshortestpaths(G, ...'Directed',
DirectedValue, ...)
[dist] = graphallshortestpaths(G, ...'Weights', WeightsValue,
    ...)
```

Arguments

G	N-by-N sparse matrix that represents a graph. Nonzero entries in matrix *G* represent the weights of the edges.
DirectedValue	Property that indicates whether the graph is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.
WeightsValue	Column vector that specifies custom weights for the edges in matrix *G*. It must have one entry for every nonzero value (edge) in matrix *G*. The order of the custom weights in the vector must match the order of the nonzero values in matrix *G* when it is traversed column-wise. This property lets you use zero-valued weights. By default, `graphallshortestpaths` gets weight information from the nonzero entries in matrix *G*.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`[dist] = graphallshortestpaths(G)` finds the shortest paths between every pair of nodes in the graph represented by matrix *G*, using Johnson's algorithm. Input *G* is an N-by-N sparse matrix that represents a graph. Nonzero entries in matrix *G* represent the weights of the edges.

Output *dist* is an N-by-N matrix where *dist*(S,T) is the distance of the shortest path from node S to node T. A 0 in this matrix indicates the source node; an Inf is an unreachable node. The *pred* output is the predecessor map of the winning paths.

Johnson's algorithm has a time complexity of O(N*log(N)+N*E), where N and E are the number of nodes and edges respectively.

[...] = graphallshortestpaths (*G*, '*PropertyName*', *PropertyValue*, ...) calls graphallshortestpaths with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

[*dist*] = graphallshortestpaths(*G*, ...'Directed', *DirectedValue*, ...) indicates whether the graph is directed or undirected. Set *DirectedValue* to false for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is true.

[*dist*] = graphallshortestpaths(*G*, ...'Weights', *WeightsValue*, ...) lets you specify custom weights for the edges. *WeightsValue* is a column vector having one entry for every nonzero value (edge) in matrix *G*. The order of the custom weights in the vector must match the order of the nonzero values in matrix *G* when it is traversed column-wise. This property lets you use zero-valued weights. By default, graphallshortestpaths gets weight information from the nonzero entries in matrix *G*.

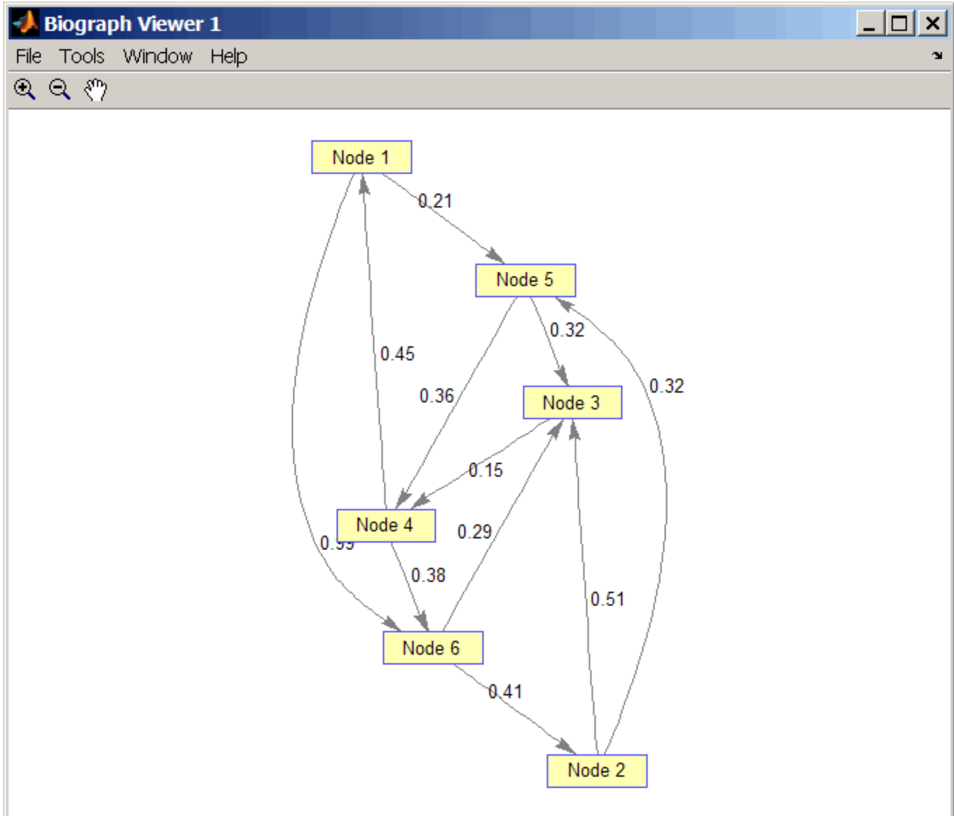
Examples

Finding All Shortest Paths in a Directed Graph

1 Create and view a directed graph with 6 nodes and 11 edges.

```
W = [.41 .99 .51 .32 .15 .45 .38 .32 .36 .29 .21];
DG = sparse([6 1 2 2 3 4 4 5 5 6 1],[2 6 3 5 4 1 6 3 4 3 5],W)

DG =
```

```
   (4,1)        0.4500
   (6,2)        0.4100
   (2,3)        0.5100
   (5,3)        0.3200
   (6,3)        0.2900
   (3,4)        0.1500
   (5,4)        0.3600
   (1,5)        0.2100
   (2,5)        0.3200
   (1,6)        0.9900
   (4,6)        0.3800

view(biograph(DG,[],'ShowWeights','on'))
```



2 Find all the shortest paths between every pair of nodes in the directed graph.

```
graphallshortestpaths(DG)

ans =

         0    1.3600    0.5300    0.5700    0.2100    0.9500
    1.1100         0    0.5100    0.6600    0.3200    1.0400
    0.6000    0.9400         0    0.1500    0.8100    0.5300
```

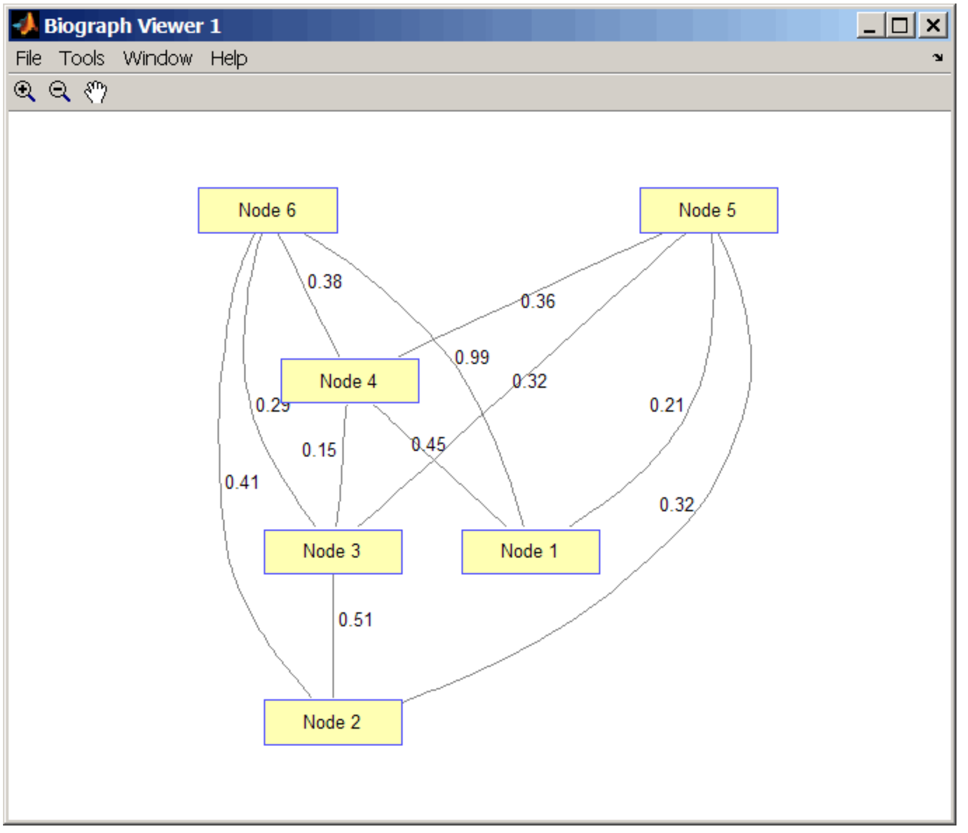
```
    0.4500    0.7900    0.6700         0    0.6600    0.3800
    0.8100    1.1500    0.3200    0.3600         0    0.7400
    0.8900    0.4100    0.2900    0.4400    0.7300         0
```

The resulting matrix shows the shortest path from node 1 (first row) to node 6 (sixth column) is 0.95. You can see this in the graph by tracing the path from node 1 to node 5 to node 4 to node 6 (0.21 + 0.36 + 0.38 = 0.95).

Finding All Shortest Paths in an Undirected Graph

1 Create and view an undirected graph with 6 nodes and 11 edges.

```
UG = tril(DG + DG')

UG =

   (4,1)        0.4500
   (5,1)        0.2100
   (6,1)        0.9900
   (3,2)        0.5100
   (5,2)        0.3200
   (6,2)        0.4100
   (4,3)        0.1500
   (5,3)        0.3200
   (6,3)        0.2900
   (5,4)        0.3600
   (6,4)        0.3800

view(biograph(UG,[],'ShowArrows','off','ShowWeights','on'))
```



2 Find all the shortest paths between every pair of nodes in the undirected graph.

```
graphallshortestpaths(UG,'directed',false)

ans =

         0    0.5300    0.5300    0.4500    0.2100    0.8300
    0.5300         0    0.5100    0.6600    0.3200    0.7000
    0.5300    0.5100         0    0.1500    0.3200    0.5300
```

```
0.4500    0.6600    0.1500         0    0.3600    0.3800
0.2100    0.3200    0.3200    0.3600         0    0.7400
0.8300    0.7000    0.5300    0.3800    0.7400         0
```

The resulting matrix is symmetrical because it represents an undirected graph. It shows the shortest path from node 1 (first row) to node 6 (sixth column) is 0.83. You can see this in the graph by tracing the path from node 1 to node 4 to node 6 (0.45 + 0. 38 = 0.83). Because `UG` is an undirected graph, we can use the edge between node 1 and node 4, which we could not do in the directed graph `DG`.

References

[1] Johnson, D.B. (1977). Efficient algorithms for shortest paths in sparse networks. Journal of the ACM *24(1)*, 1-13.

[2] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox method of `biograph object`: `allshortestpaths`

Purpose

Find strongly or weakly connected components in graph

Syntax

```
[S, C] = graphconncomp(G)
[S, C] = graphconncomp(G, ...'Directed', DirectedValue, ...)
[S, C] = graphconncomp(G, ...'Weak', WeakValue, ...)
```

Arguments

G	N-by-N sparse matrix that represents a graph. Nonzero entries in matrix `G` indicate the presence of an edge.
DirectedValue	Property that indicates whether the graph is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`. A DFS-based algorithm computes the connected components. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.
WeakValue	Property that indicates whether to find weakly connected components or strongly connected components. A weakly connected component is a maximal group of nodes that are mutually reachable by violating the edge directions. Set *WeakValue* to `true` to find weakly connected components. Default is `false`, which finds strongly connected components. The state of this parameter has no effect on undirected graphs because weakly and strongly connected components are the same in undirected graphs. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`[S, C] = graphconncomp(G)` finds the strongly connected components of the graph represented by matrix `G` using Tarjan's algorithm. A strongly connected component is a maximal group of nodes that are mutually reachable without violating the edge directions. Input `G` is an N-by-N sparse matrix that represents a graph. Nonzero entries in matrix `G` indicate the presence of an edge.

The number of components found is returned in `S`, and `C` is a vector indicating to which component each node belongs.

Tarjan's algorithm has a time complexity of `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively.

`[S, C] = graphconncomp(G, ...'PropertyName', PropertyValue, ...)` calls `graphconncomp` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[S, C] = graphconncomp(G, ...'Directed', DirectedValue, ...)` indicates whether the graph is directed or undirected. Set *directedValue* to `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`. A DFS-based algorithm computes the connected components. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

`[S, C] = graphconncomp(G, ...'Weak', WeakValue, ...)` indicates whether to find weakly connected components or strongly connected components. A weakly connected component is a maximal group of nodes that are mutually reachable by violating the edge directions. Set *WeakValue* to `true` to find weakly connected components. Default is `false`, which finds strongly connected components. The state of this parameter has no effect on undirected graphs because weakly and strongly connected components are the same in undirected graphs. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

Note By definition, a single node can be a strongly connected component.

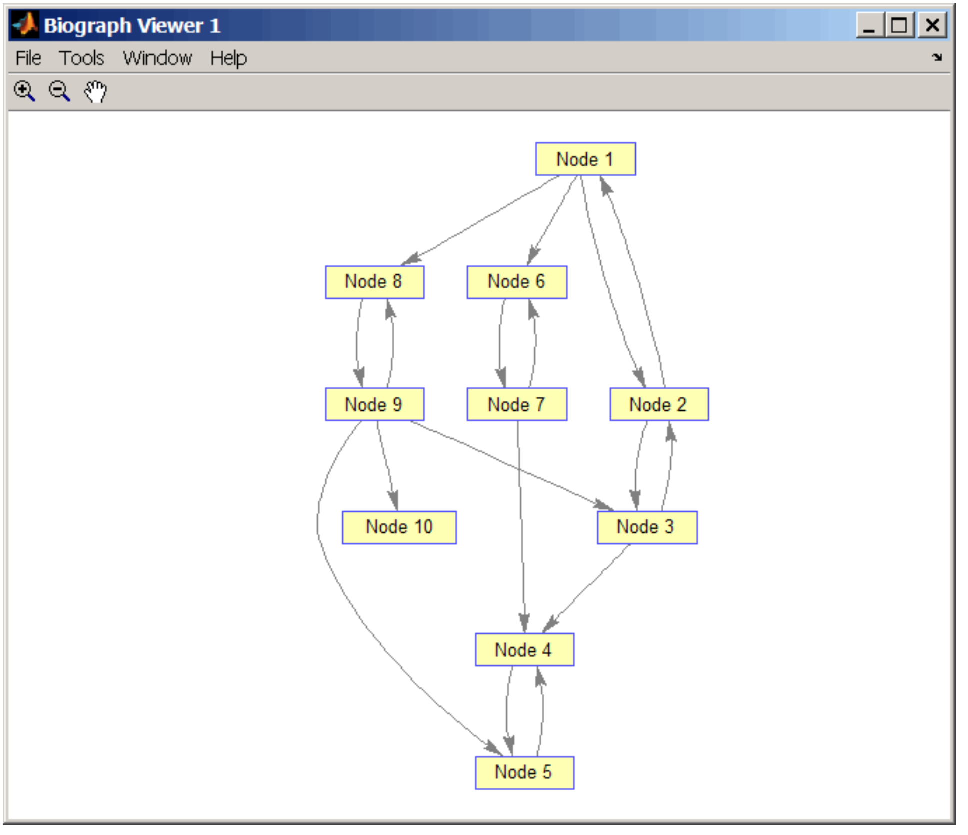
Note A directed acyclic graph (DAG) cannot have any strongly connected components larger than one.

Examples

1 Create and view a directed graph with 10 nodes and 17 edges.

```
DG = sparse([1 1 1 2 2 3 3 4 5 6 7 7 8 9 9  9 9], ...
            [2 6 8 3 1 4 2 5 4 7 6 4 9 8 10 5 3],true,10,10)

DG =

   (2,1)        1
   (1,2)        1
   (3,2)        1
   (2,3)        1
   (9,3)        1
   (3,4)        1
   (5,4)        1
   (7,4)        1
   (4,5)        1
   (9,5)        1
   (1,6)        1
   (7,6)        1
   (6,7)        1
   (1,8)        1
   (9,8)        1
```

```
    (8,9)        1
    (9,10)       1

h = view(biograph(DG));
```



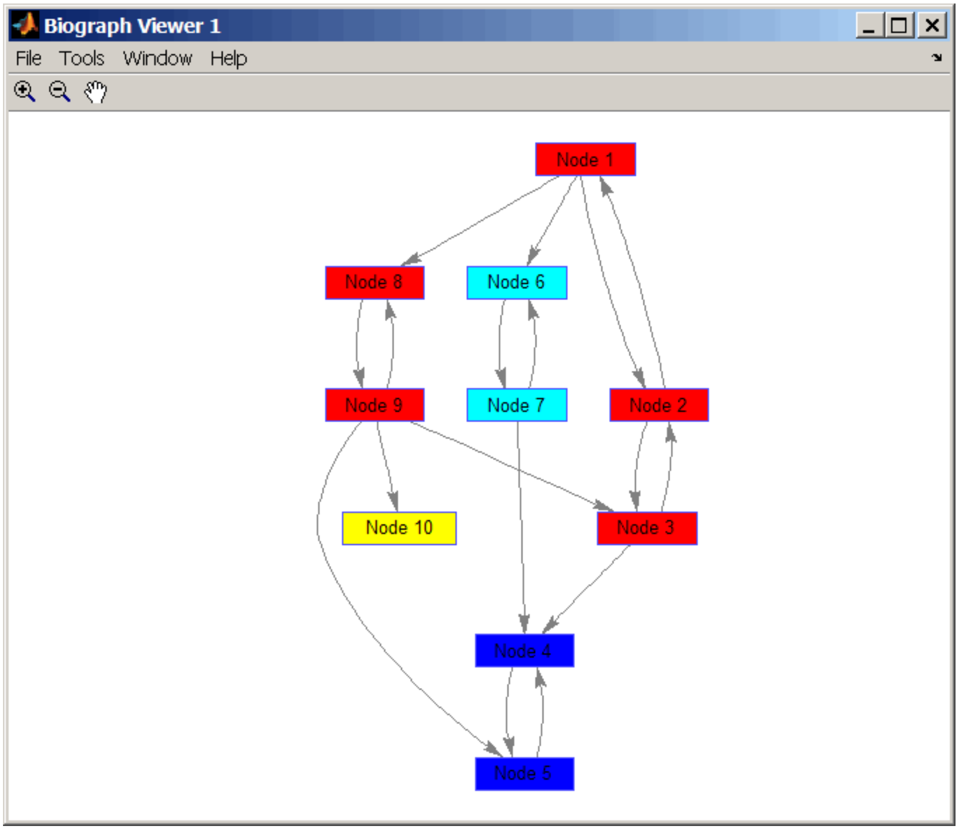
2 Find the number of strongly connected components in the directed graph and determine to which component each of the 10 nodes belongs.

```
[S,C] = graphconncomp(DG)
```

```
S =

     4


C =

     4     4     4     1     1     2     2     4     4     3
```

3 Color the nodes for each component with a different color.

```
colors = jet(S);
for i = 1:numel(h.nodes)
  h.Nodes(i).Color = colors(C(i),:);
end
```



References

[1] Tarjan, R.E., (1972). Depth first search and linear graph algorithms. SIAM Journal on Computing *1(2)*, 146–160.

[2] Sedgewick, R., (2002). Algorithms in C++, Part 5 Graph Algorithms (Addison-Wesley).

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox method of `biograph object`: `conncomp`

Purpose

Test for cycles in directed graph

Syntax

`graphisdag(G)`

Arguments

G	N-by-N sparse matrix that represents a directed graph. Nonzero entries in matrix *G* indicate the presence of an edge.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`graphisdag(G)` returns logical 1 (`true`) if the directed graph represented by matrix *G* is a directed acyclic graph (DAG) and logical 0 (`false`) otherwise. *G* is an N-by-N sparse matrix that represents a directed graph. Nonzero entries in matrix *G* indicate the presence of an edge.

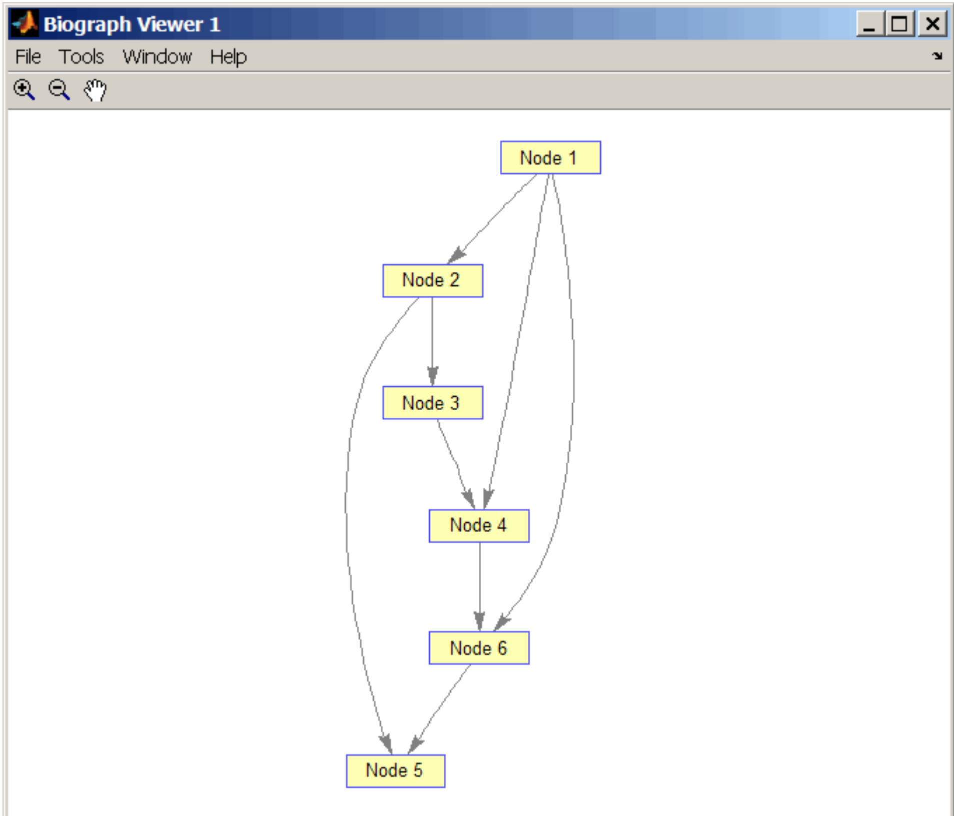
Examples

Testing for Cycles in Directed Graphs

1 Create and view a directed acyclic graph (DAG) with six nodes and eight edges.

```
DG = sparse([1 1 1 2 2 3 4 6],[2 4 6 3 5 4 6 5],true,6,6)

DG =

   (1,2)        1
   (2,3)        1
   (1,4)        1
   (3,4)        1
   (2,5)        1
   (6,5)        1
   (1,6)        1
   (4,6)        1
```

```
view(biograph(DG))
```

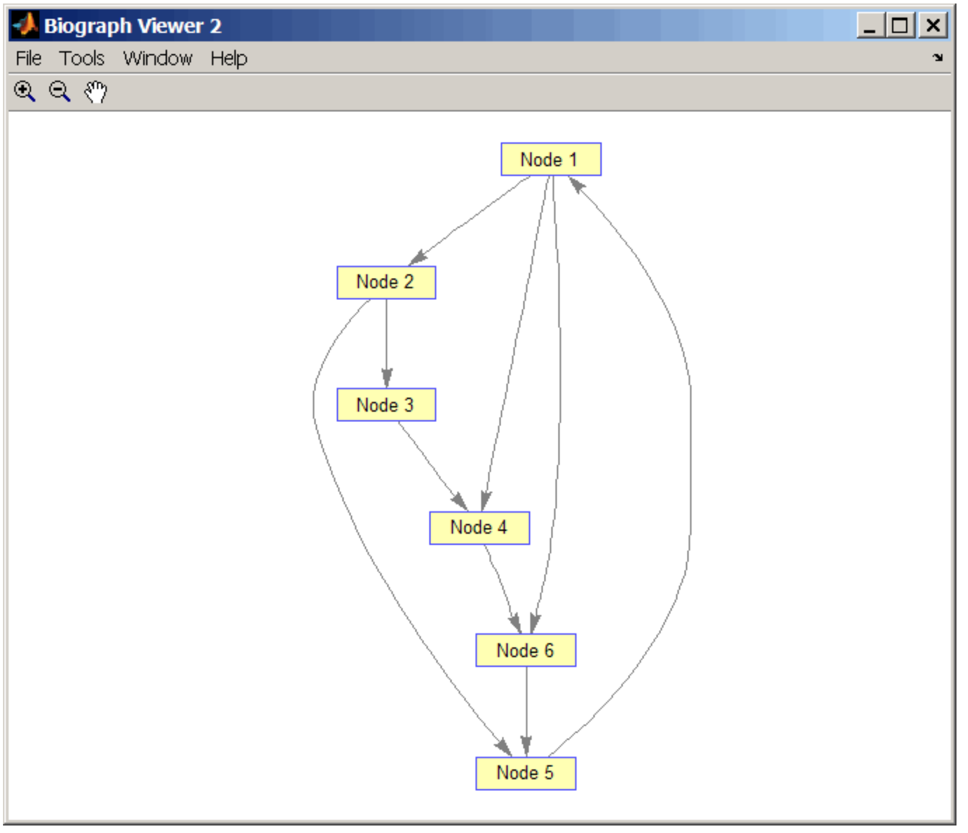


2 Test for cycles in the DAG.

```
graphisdag(DG)

ans =

     1
```

3 Add an edge to the DAG to make it cyclic, and then view the directed graph.

```
DG(5,1) = true

DG =

   (5,1)        1
   (1,2)        1
   (2,3)        1
   (1,4)        1
   (3,4)        1
   (2,5)        1
   (6,5)        1
   (1,6)        1
   (4,6)        1

>> view(biograph(DG))
```



4 Test for cycles in the new graph.

```
graphisdag(DG)

ans =

     0
```

Testing for Cycles in a Very Large Graph (Greater Than 20,000 Nodes and 30,000 Edges)

1 Download the Gene Ontology database to a geneont object.

```
GO = geneont('live',true);
```

2 Convert the geneont object to a matrix.

```
CM = getmatrix(GO);
```

3 Test for cycles in the graph.

```
graphisdag(CM)
```

Creating a Random DAG

1 Create and view a random directed acyclic graph (DAG) with 15 nodes and 20 edges.

```
g = sparse([],[],true,15,15);
while nnz(g) < 20
  edge = randsample(15*15,1); % get a random edge
  g(edge) = true;
  g(edge) = graphisdag(g);
end
view(biograph(g))
```

2 Test for cycles in the graph.

```
graphisdag(g)
```

References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, graphminspantree, graphpred2path, graphshortestpath, graphtopoorder, graphtraverse

Bioinformatics Toolbox method of biograph object: isdag

Purpose

Find isomorphism between two graphs

Syntax

```
[Isomorphic, Map] = graphisomorphism(G1, G2)
[Isomorphic, Map] = graphisomorphism(G1, G2,'Directed',
    DirectedValue)
```

Arguments

G1	N-by-N sparse matrix that represents a directed or undirected graph. Nonzero entries in matrix *G1* indicate the presence of an edge.
G2	N-by-N sparse matrix that represents a directed or undirected graph. *G2* must be the same (directed or undirected) as *G1*.
DirectedValue	Property that indicates whether the graphs are directed or undirected. Enter `false` when both *G1* and *G2* are undirected graphs. In this case, the upper triangles of the sparse matrices *G1* and *G2* are ignored. Default is `true`, meaning that both graphs are directed.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`[Isomorphic, Map] = graphisomorphism(G1, G2)` returns logical 1 (`true`) in *Isomorphic* if *G1* and *G2* are isomorphic graphs, and logical 0 (`false`) otherwise. A graph isomorphism is a 1-to-1 mapping of the nodes in the graph *G1* and the nodes in the graph *G2* such that adjacencies are preserved. *G1* and *G2* are both N-by-N sparse matrices that represent directed or undirected graphs. Return value *Isomorphic* is Boolean. When *Isomorphic* is `true`, *Map* is a row vector containing the node indices that map from *G2* to *G1*. When *Isomorphic* is `false`, the worst-case time complexity is `O(N!)`, where `N` is the number of nodes.

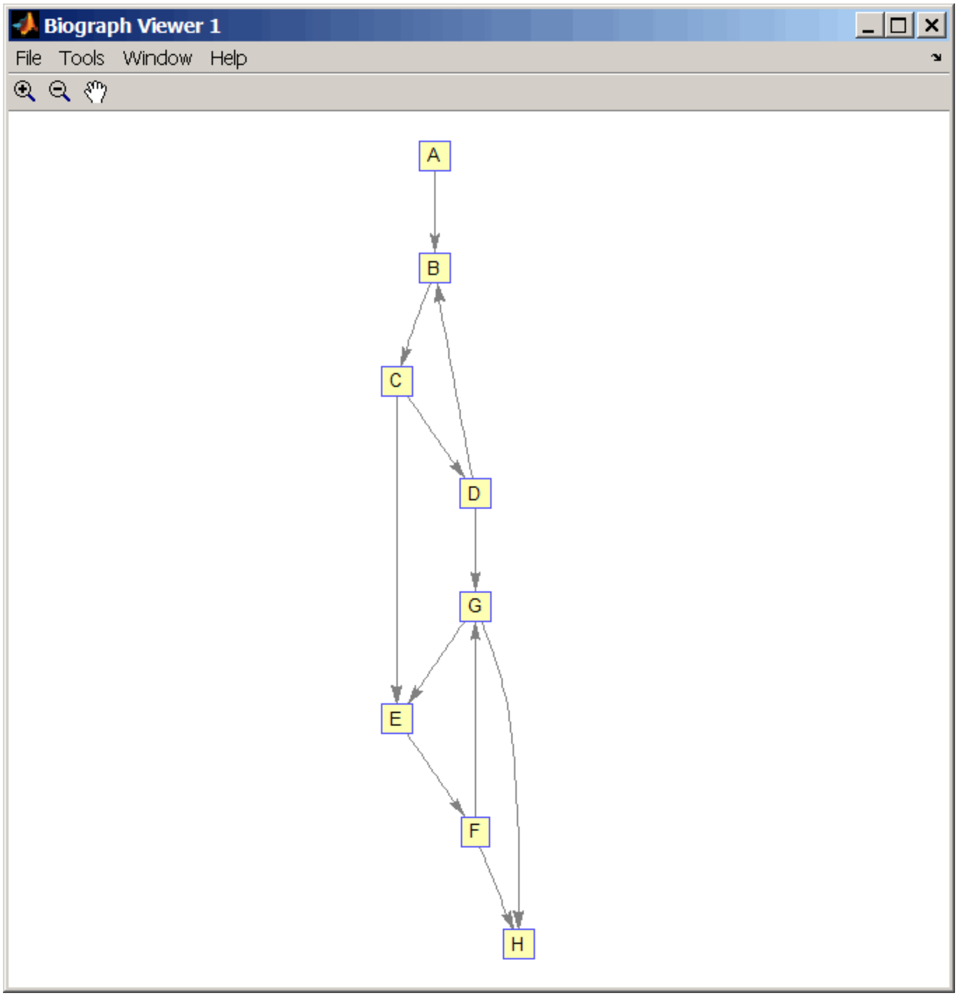
graphisomorphism

`[Isomorphic, Map] = graphisomorphism(G1, G2,'Directed', DirectedValue)` indicates whether the graphs are directed or undirected. Set `DirectedValue` to `false` when both `G1` and `G2` are undirected graphs. In this case, the upper triangles of the sparse matrices `G1` and `G2` are ignored. Default is `true`, meaning that both graphs are directed.

Examples

1 Create and view a directed graph with 8 nodes and 11 edges.

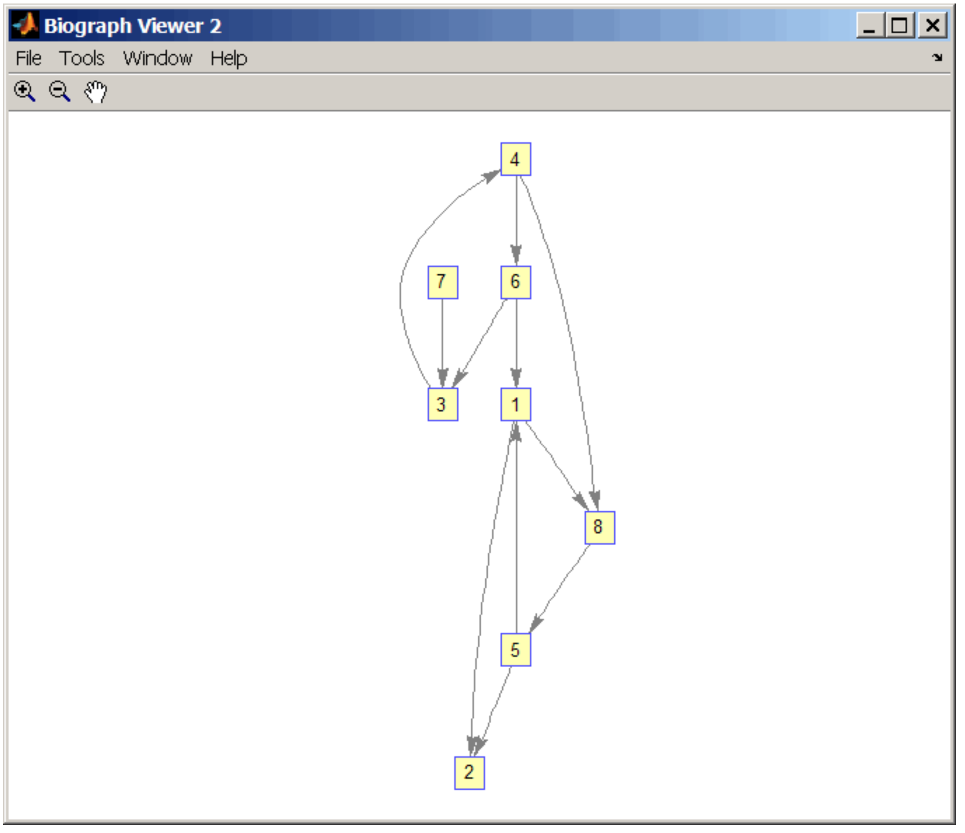
```
m('ABCDEFGH') = [1 2 3 4 5 6 7 8];
g1 = sparse(m('ABDCDCGEFFG'),m('BCBDGEEFHGH'),true,8,8)

g1 =

   (1,2)        1
   (4,2)        1
   (2,3)        1
   (3,4)        1
   (3,5)        1
   (7,5)        1
   (5,6)        1
   (4,7)        1
   (6,7)        1
   (6,8)        1
   (7,8)        1

view(biograph(g1,'ABCDEFGH'))
```



2 Set a random permutation vector and then create and view a new permuted graph.

```
p = randperm(8)
```

```
p =

     7     8     2     3     6     4     1     5

g2 = g1(p,p);
view(biograph(g2,'12345678'))
```



3 Check if the two graphs are isomorphic.

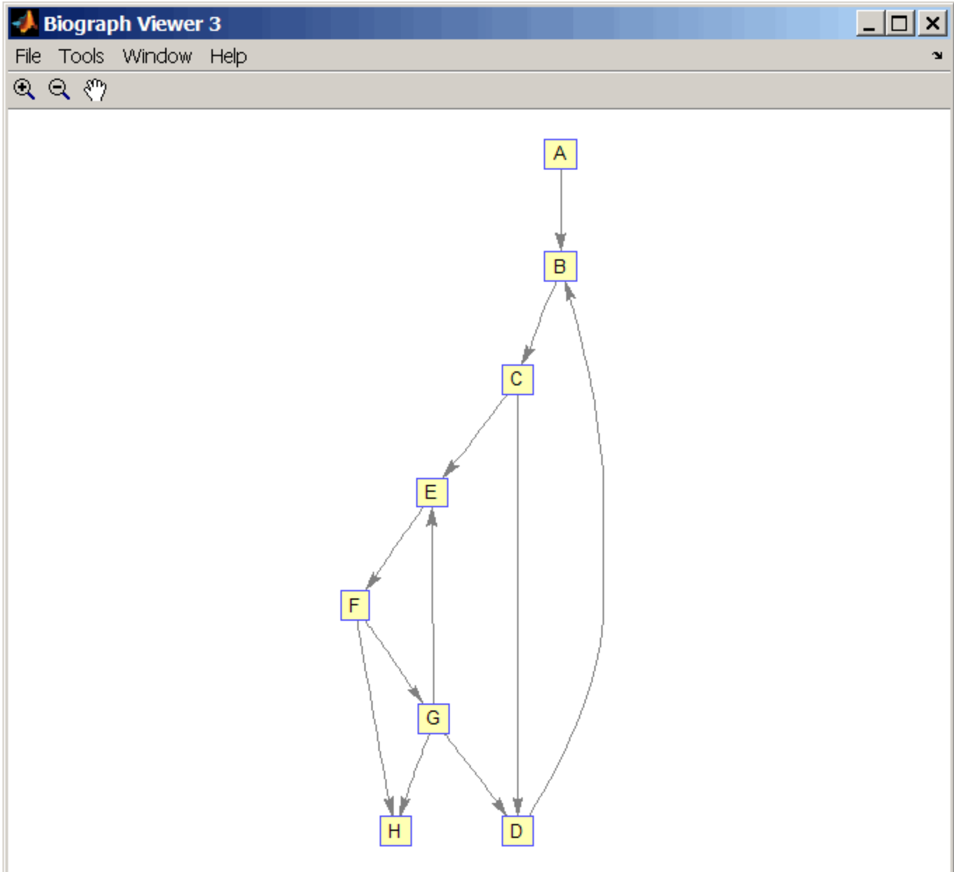
```
[F,Map] = graphisomorphism(g2,g1)
```

```
F =

     1


Map =

     7     8     2     3     6     4     1     5
```

Note that the Map row vector containing the node indices that map from g2 to g1 is the same as the permutation vector you created in step 2.

4 Reverse the direction of the D-G edge in the first graph, and then check for isomorphism again.

```
g1(m('DG'),m('GD')) = g1(m('GD'),m('DG'));
view(biograph(g1,'ABCDEFGH'))
```




```
[F,M] = graphisomorphism(g2,g1)

F =

     0


M =
```

```
    []
```

5 Convert the graphs to undirected graphs, and then check for isomorphism.

```
[F,M] = graphisomorphism(g2+g2',g1+g1','directed',false)

F =

     1


M =

     7     8     2     3     6     4     1     5
```

References

[1] Fortin, S. (1996). The Graph Isomorphism Problem. Technical Report, 96-20, Dept. of Computer Science, University of Alberta, Edomonton, Alberta, Canada.

[2] McKay, B.D. (1981). Practical Graph Isomorphism. Congressus Numerantium *30*, 45-87.

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox methods of `biograph object`: `isomorphism`

graphisspantree

Purpose

Determine if tree is spanning tree

Syntax

`TF = graphisspantree(G)`

Arguments

`G`	N-by-N sparse matrix whose lower triangle represents an undirected graph. Nonzero entries in matrix `G` indicate the presence of an edge.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`TF = graphisspantree(G)` returns logical 1 (`true`) if `G` is a spanning tree, and logical 0 (`false`) otherwise. A spanning tree must touch all the nodes and must be acyclic. `G` is an N-by-N sparse matrix whose lower triangle represents an undirected graph. Nonzero entries in matrix `G` indicate the presence of an edge.

Examples

1 Create a phytree object from a phylogenetic tree file.

```
tr = phytreeread('pf00002.tree')
 Phylogenetic tree object with 33 leaves (32 branches)
```

2 Create a connection matrix from the phytree object.

```
[CM,labels,dist] = getmatrix(tr);
```

3 Determine if the connection matrix is a spanning tree.

```
graphisspantree(CM)

ans =

     1
```

4 Add an edge between the root and the first leaf in the connection matrix.

```
CM(end,1) = 1;
```

5 Determine if the modified connection matrix is a spanning tree.

```
graphisspantree(CM)

ans =

     0
```

References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox methods of `biograph object`: `isspantree`

Purpose

Calculate maximum flow and minimum cut in directed graph

Syntax

```
[MaxFlow, FlowMatrix, Cut] = graphmaxflow(G, SNode, TNode)
[...] = graphmaxflow(G, SNode, TNode, ...'Capacity',
CapacityValue, ...)
[...] = graphmaxflow(G, SNode, TNode, ...'Method', MethodValue,
    ...)
```

Arguments

G	N-by-N sparse matrix that represents a directed graph. Nonzero entries in matrix `G` represent the capacities of the edges.
SNode	Node in *G*.
TNode	Node in *G*.
CapacityValue	Column vector that specifies custom capacities for the edges in matrix *G*. It must have one entry for every nonzero value (edge) in matrix *G*. The order of the custom capacities in the vector must match the order of the nonzero values in matrix *G* when it is traversed column-wise. By default, `graphmaxflow` gets capacity information from the nonzero entries in matrix *G*.
MethodValue	String that specifies the algorithm used to find the minimal spanning tree (MST). Choices are: • `'Edmonds'` — Uses the Edmonds and Karp algorithm, the implementation of which is based on a variation called the *labeling algorithm*. Time complexity is `O(N*E^2)`, where `N` and `E` are the number of nodes and edges respectively. • `'Goldberg'` — Default algorithm. Uses the Goldberg algorithm, which uses the generic method known as *preflow-push*. Time complexity is `O(N^2*sqrt(E))`, where `N` and `E` are the number of nodes and edges respectively.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`[MaxFlow, FlowMatrix, Cut] = graphmaxflow(G, SNode, TNode)` calculates the maximum flow of directed graph `G` from node `SNode` to node `TNode`. Input `G` is an N-by-N sparse matrix that represents a directed graph. Nonzero entries in matrix `G` represent the capacities of the edges. Output `MaxFlow` is the maximum flow, and `FlowMatrix` is a sparse matrix with all the flow values for every edge. `FlowMatrix(X,Y)` is the flow from node `X` to node `Y`. Output `Cut` is a logical row vector indicating the nodes connected to `SNode` after calculating the minimum cut between `SNode` and `TNode`. If several solutions to the minimum cut problem exist, then `Cut` is a matrix.

`[...] = graphmaxflow(G, SNode, TNode, ...'PropertyName', PropertyValue, ...)` calls `graphmaxflow` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[...] = graphmaxflow(G, SNode, TNode, ...'Capacity', CapacityValue, ...)` lets you specify custom capacities for the edges. `CapacityValue` is a column vector having one entry for every nonzero value (edge) in matrix `G`. The order of the custom capacities in the vector must match the order of the nonzero values in matrix `G` when it is traversed column-wise. By default, `graphmaxflow` gets capacity information from the nonzero entries in matrix `G`.

`[...] = graphmaxflow(G, SNode, TNode, ...'Method', MethodValue, ...)` lets you specify the algorithm used to find the minimal spanning tree (MST). Choices are:

- `'Edmonds'` — Uses the Edmonds and Karp algorithm, the implementation of which is based on a variation called the *labeling* *algorithm*. Time complexity is `O(N*E^2)`, where `N` and `E` are the number of nodes and edges respectively.

- `'Goldberg'` — Default algorithm. Uses the Goldberg algorithm, which uses the generic method known as *preflow-push*. Time complexity is `O(N^2*sqrt(E))`, where `N` and `E` are the number of nodes and edges respectively.

Examples

1 Create a directed graph with six nodes and eight edges.

```
cm = sparse([1 1 2 2 3 3 4 5],[2 3 4 5 4 5 6 6],...
     [2 3 3 1 1 1 2 3],6,6)
cm =

   (1,2)        2
   (1,3)        3
   (2,4)        3
   (3,4)        1
   (2,5)        1
   (3,5)        1
   (4,6)        2
   (5,6)        3
```

2 Calculate the maximum flow in the graph from node 1 to node 6.

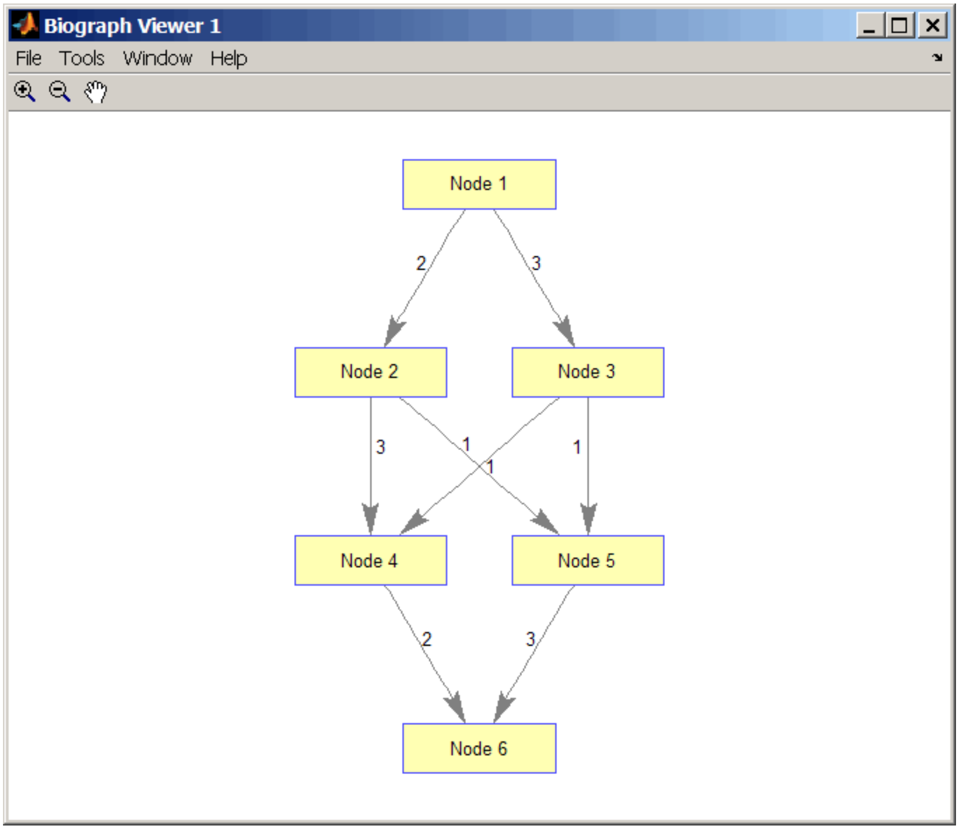
```
[M,F,K] = graphmaxflow(cm,1,6)

M =

     4


F =

   (1,2)        2
   (1,3)        2
   (2,4)        1
   (3,4)        1
```

```
    (2,5)        1
    (3,5)        1
    (4,6)        2
    (5,6)        2


K =

     1     1     1     1     0     0
     1     0     1     0     0     0
```

Notice that `K` is a two-row matrix because there are two possible solutions to the minimum cut problem.

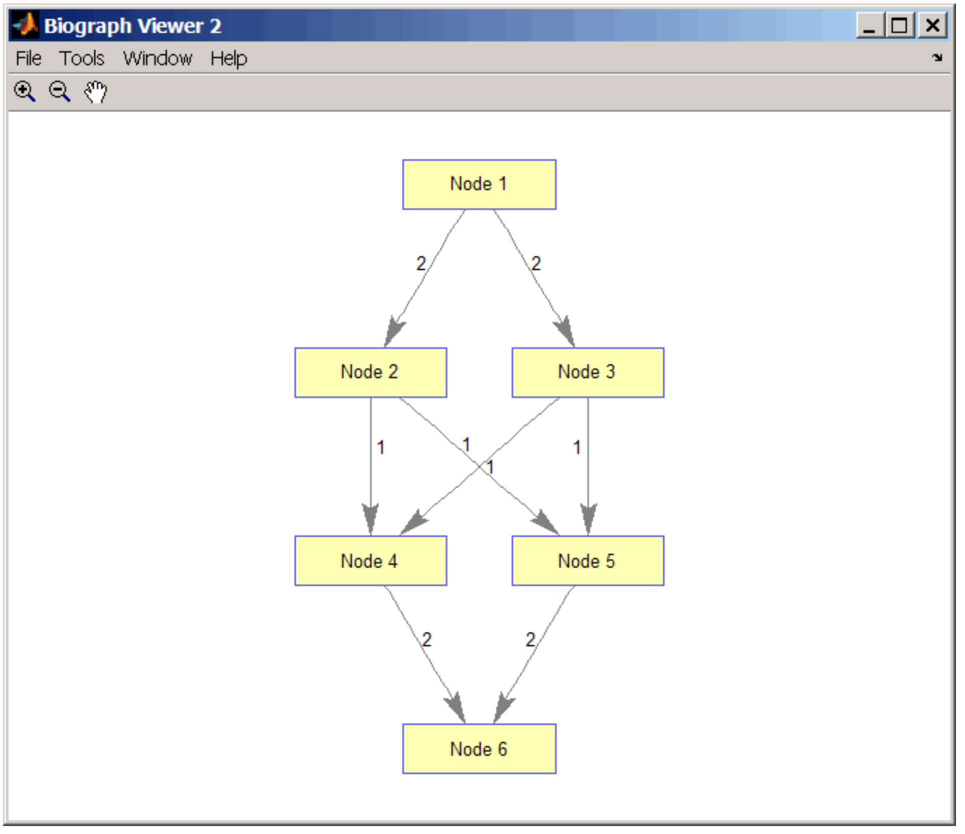
3 View the graph with the original capacities.

```
h = view(biograph(cm,[],'ShowWeights','on'))
```



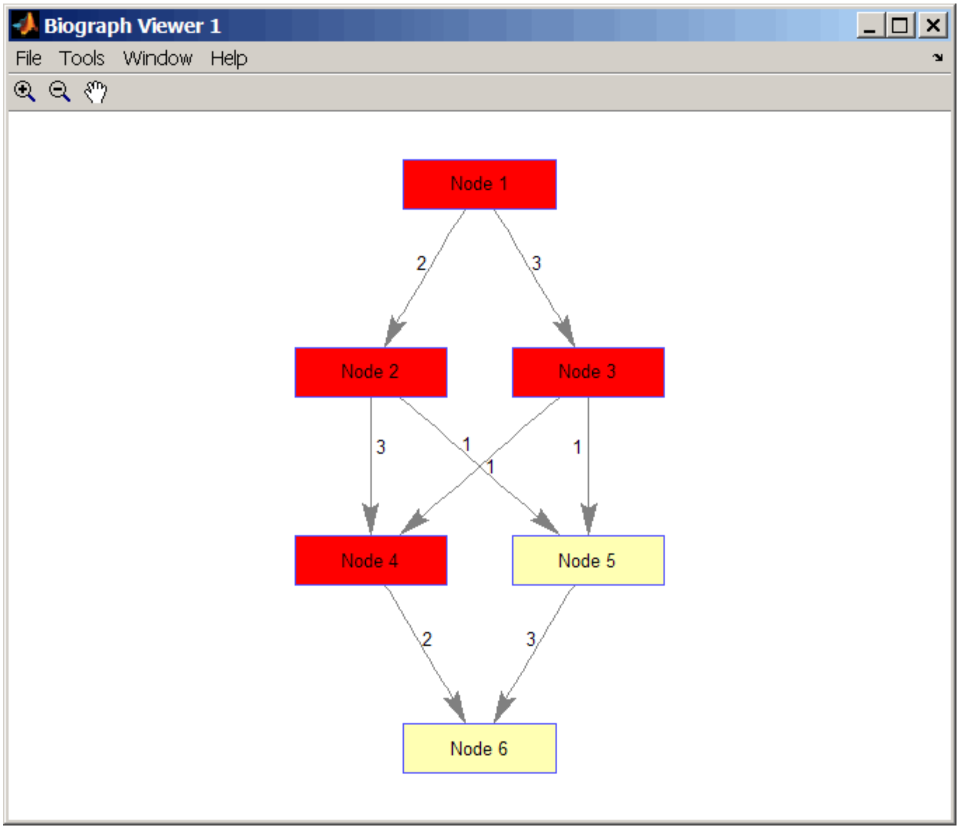
4 View the graph with the calculated maximum flows.

```
view(biograph(F,[],'ShowWeights','on'))
```



5 Show one solution to the minimum cut problem in the original graph.

```
set(h.Nodes(K(1,:)),'Color',[1 0 0])
```



Notice that in the three edges that connect the source nodes (red) to the destination nodes (yellow), the original capacities and the calculated maximum flows are the same.

References

[1] Edmonds, J. and Karp, R.M. (1972). Theoretical improvements in the algorithmic efficiency for network flow problems. Journal of the ACM *19*, 248-264.

[2] Goldberg, A.V. (1985). A New Max-Flow Algorithm. MIT Technical Report MIT/LCS/TM-291, Laboratory for Computer Science, MIT.

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox method of `biograph object`: `maxflow`

graphminspantree

Purpose

Find minimal spanning tree in graph

Syntax

```
[Tree, pred] = graphminspantree(G)
[Tree, pred] = graphminspantree(G, R)
[Tree, pred] = graphminspantree(..., 'Method', MethodValue, ...)
[Tree, pred] = graphminspantree(..., 'Weights', WeightsValue,
    ...)
```

Arguments

G	N-by-N sparse matrix that represents an undirected graph. Nonzero entries in matrix *G* represent the weights of the edges.
R	Scalar between 1 and the number of nodes.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`[Tree, pred] = graphminspantree(G)` finds an acyclic subset of edges that connects all the nodes in the undirected graph *G* and for which the total weight is minimized. Weights of the edges are all nonzero entries in the lower triangle of the N-by-N sparse matrix *G*. Output *Tree* is a spanning tree represented by a sparse matrix. Output *pred* is a vector containing the predecessor nodes of the minimal spanning tree (MST), with the root node indicated by `0`. The root node defaults to the first node in the largest connected component. This computation requires an extra call to the `graphconncomp` function.

`[Tree, pred] = graphminspantree(G, R)` sets the root of the minimal spanning tree to node `R`.

`[Tree, pred] = graphminspantree(..., 'PropertyName', PropertyValue, ...)` calls `graphminspantree` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[Tree, pred] = graphminspantree(..., 'Method', MethodValue, ...)` lets you specify the algorithm used to find the minimal spanning tree (MST). Choices are:

- `'Kruskal'` — Grows the minimal spanning tree (MST) one edge at a time by finding an edge that connects two trees in a spreading forest of growing MSTs. Time complexity is `O(E+X*log(N))`, where `X` is the number of edges no longer than the longest edge in the MST, and `N` and `E` are the number of nodes and edges respectively.
- `'Prim'` — Default algorithm. Grows the minimal spanning tree (MST) one edge at a time by adding a minimal edge that connects a node in the growing MST with any other node. Time complexity is `O(E*log(N))`, where `N` and `E` are the number of nodes and edges respectively.

Note When the graph is unconnected, Prim's algorithm returns only the tree that contains R, while Kruskal's algorithm returns an MST for every component.

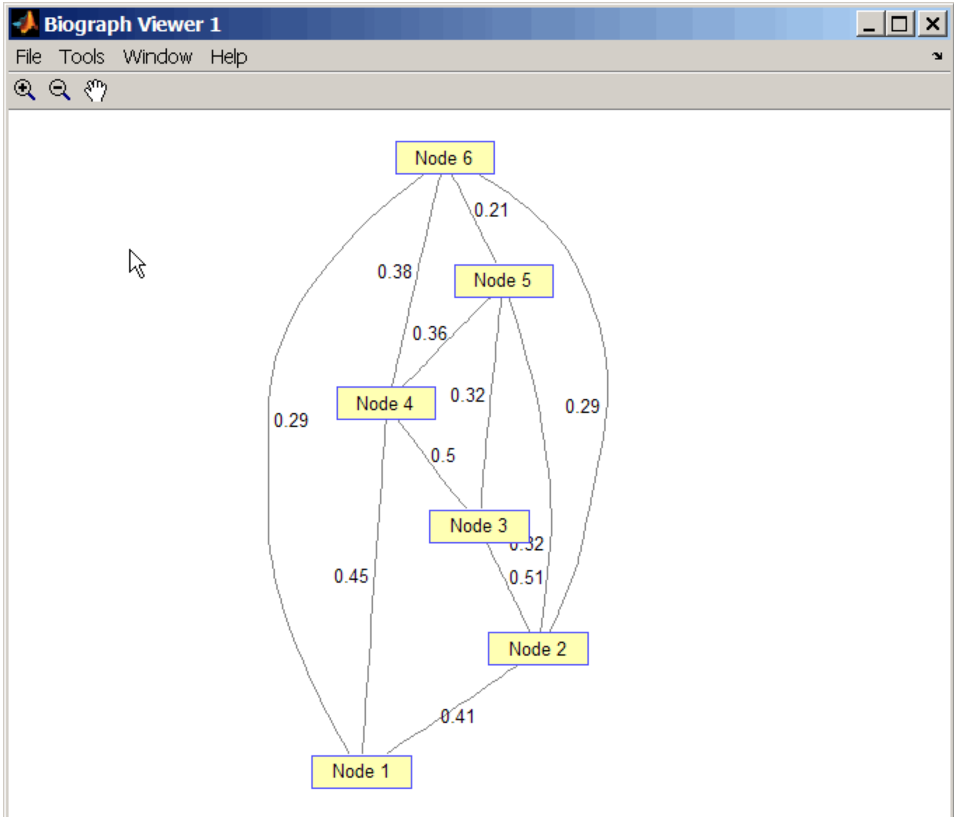
`[Tree, pred] = graphminspantree(..., 'Weights', WeightsValue, ...)` lets you specify custom weights for the edges. *`WeightsValue`* is a column vector having one entry for every nonzero value (edge) in matrix *G*. The order of the custom weights in the vector must match the order of the nonzero values in matrix *G* when it is traversed column-wise. By default, `graphminspantree` gets weight information from the nonzero entries in matrix *G*.

Examples

1 Create and view an undirected graph with 6 nodes and 11 edges.

```
W = [.41 .29 .51 .32 .50 .45 .38 .32 .36 .29 .21];
DG = sparse([1 1 2 2 3 4 4 5 5 6 6],[2 6 3 5 4 1 6 3 4 2 5],W);
```

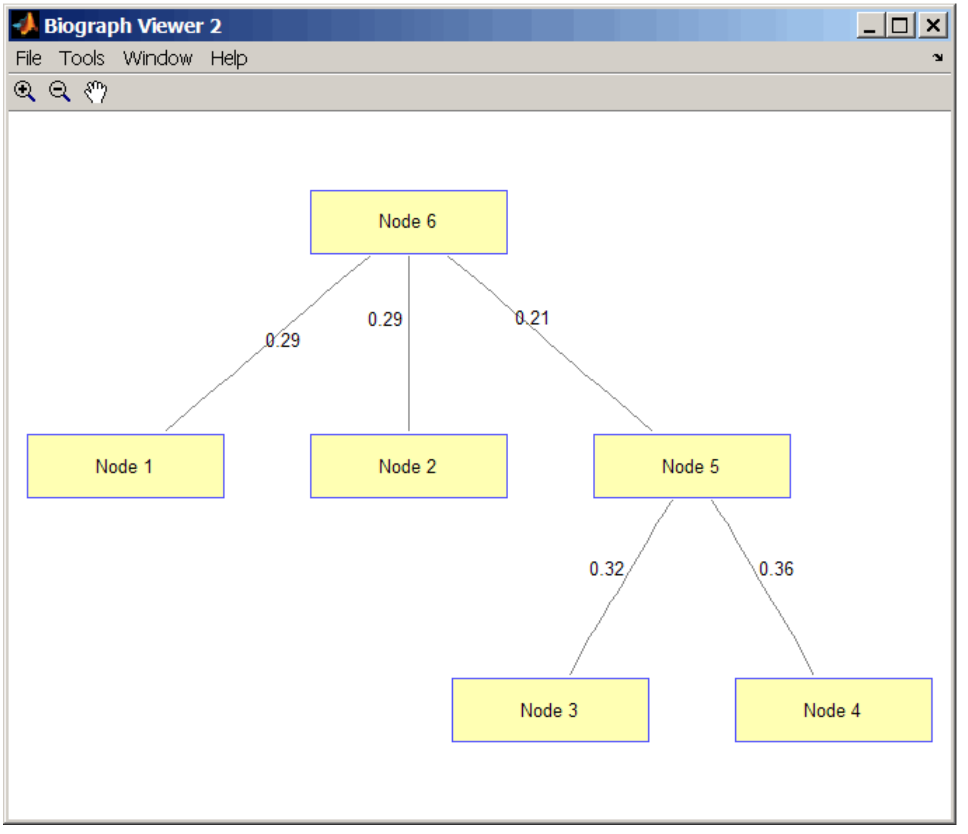
```
UG = tril(DG + DG')

UG =

   (2,1)       0.4100
   (4,1)       0.4500
   (6,1)       0.2900
   (3,2)       0.5100
   (5,2)       0.3200
   (6,2)       0.2900
   (4,3)       0.5000
   (5,3)       0.3200
   (5,4)       0.3600
   (6,4)       0.3800
   (6,5)       0.2100

view(biograph(UG,[],'ShowArrows','off','ShowWeights','on'))
```



2 Find and view the minimal spanning tree of the undirected graph.

```
[ST,pred] = graphminspantree(UG)

ST =

    (6,1)        0.2900
    (6,2)        0.2900
    (5,3)        0.3200
    (5,4)        0.3600
```

```
   (6,5)        0.2100


pred =

     0     6     5     5     6     1

view(biograph(ST,[],'ShowArrows','off','ShowWeights','on'))
```



References

[1] Kruskal, J.B. (1956). On the Shortest Spanning Subtree of a Graph and the Traveling Salesman Problem. Proceedings of the American Mathematical Society *7*, 48-50.

[2] Prim, R. (1957). Shortest Connection Networks and Some Generalizations. Bell System Technical Journal *36*, 1389-1401.

[3] Siek, J.G. Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox method of `biograph object`: `minspantree`

graphpred2path

Purpose

Convert predecessor indices to paths

Syntax

`path = graphpred2path(pred, D)`

Arguments

pred	Row vector or matrix of predecessor node indices. The value of the root (or source) node in *pred* must be 0.
D	Destination node in *pred*.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`path = graphpred2path(pred, D)` traces back a path by following the predecessor list in *pred* starting at destination node *D*.

The value of the root (or source) node in *pred* must be 0. If a NaN is found when following the predecessor nodes, `graphpred2path` returns an empty path.

If *pred* is a ...	And *D* is a ...	Then *path* is a ...
row vector of predecessor node indices	scalar	row vector listing the nodes from the root (or source) to *D*.
	row vector	row cell array with every column containing the path to the destination for every element in *D*.

If *pred* is a ...	And *D* is a ...	Then *path* is a ...
matrix	scalar	column cell array with every row containing the path for every row in *pred*.
	row vector	matrix cell array with every row containing the paths for the respective row in *pred*, and every column containing the paths to the respective destination in *D*.

Note If *D* is omitted, the paths to all the destinations are calculated for every predecessor listed in *pred*.

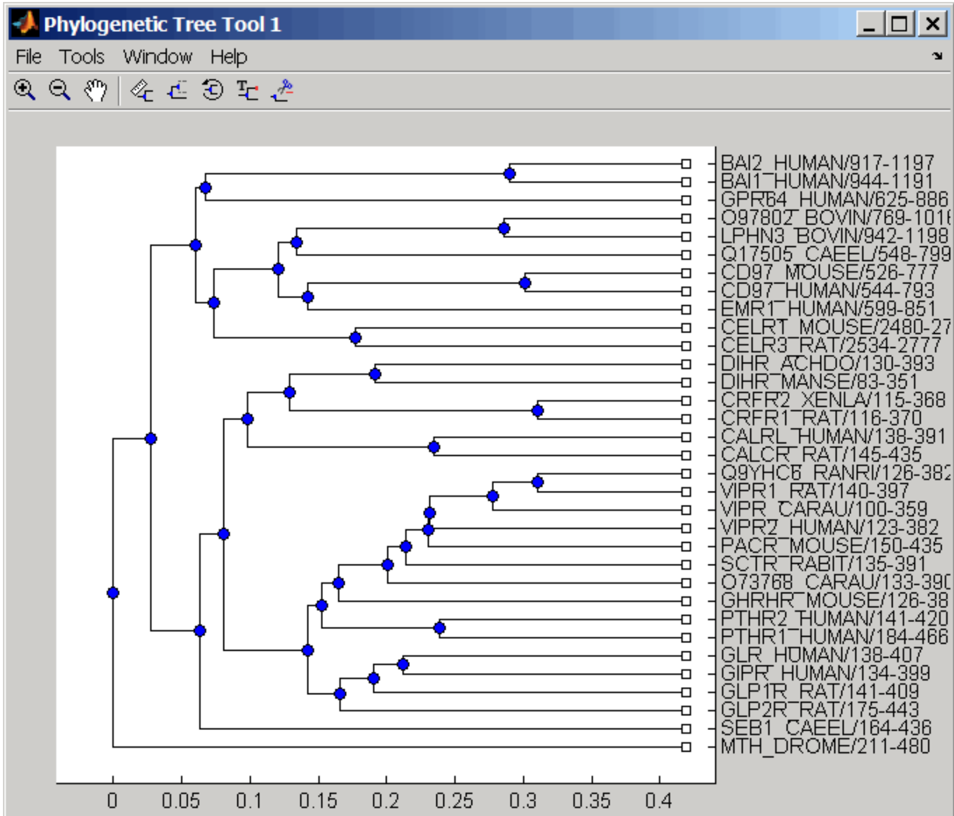
Examples

1. Create a phytree object from the phylogenetic tree file for the GLR_HUMAN protein.

```
tr = phytreeread('pf00002.tree')
    Phylogenetic tree object with 33 leaves (32 branches)
```

2. View the phytree object.

```
view(tr)
```



3 From the phytree object, create a connection matrix to represent the phylogenetic tree.

```
[CM,labels,dist] = getmatrix(tr);
```

4 Find the nodes from the root to one leaf in the phylogenetic tree created from the phylogenetic tree file for the GLR_HUMAN protein.

```
root_loc = size(CM,1)

root_loc =
```

```
    65

glr_loc = strmatch('GLR',labels)

glr_loc =

    28

[T,PRED]=graphminspantree(CM,root_loc);
PATH = graphpred2path(PRED,glr_loc)

PATH =

    65    64    53    52    46    45    44    43    28
```

References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

graphshortestpath

Purpose

Solve shortest path problem in graph

Syntax

```
[dist, path, pred] = graphshortestpath(G, S)
[dist, path, pred] = graphshortestpath(G, S, T)
[...] = graphshortestpath(..., 'Directed', DirectedValue, ...)
[...] = graphshortestpath(..., 'Method', MethodValue, ...)
[...] = graphshortestpath(..., 'Weights', WeightsValue, ...)
```

Arguments

G	N-by-N sparse matrix that represents a graph. Nonzero entries in matrix *G* represent the weights of the edges.
S	Node in *G*.
T	Node in *G*.
DirectedValue	Property that indicates whether the graph is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.

MethodValue	String that specifies the algorithm used to find the shortest path. Choices are: • `'Bellman-Ford'` — Assumes weights of the edges to be nonzero entries in sparse matrix `G`. Time complexity is `O(N*E)`, where `N` and `E` are the number of nodes and edges respectively. • `'BFS'` — Breadth-first search. Assumes all weights to be equal, and nonzero entries in sparse matrix `G` to represent edges. Time complexity is `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively. • `'Acyclic'` — Assumes `G` to be a directed acyclic graph and that weights of the edges are nonzero entries in sparse matrix `G`. Time complexity is `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively. • `'Dijkstra'` — Default algorithm. Assumes weights of the edges to be positive values in sparse matrix `G`. Time complexity is `O(log(N)*E)`, where `N` and `E` are the number of nodes and edges respectively.
WeightsValue	Column vector that specifies custom weights for the edges in matrix *`G`*. It must have one entry for every nonzero value (edge) in matrix *`G`*. The order of the custom weights in the vector must match the order of the nonzero values in matrix *`G`* when it is traversed column-wise. This property lets you use zero-valued weights. By default, `graphshortestpaths` gets weight information from the nonzero entries in matrix *`G`*.

graphshortestpath

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`[dist, path, pred] = graphshortestpath(G, S)` determines the single-source shortest paths from node `S` to all other nodes in the graph represented by matrix `G`. Input `G` is an N-by-N sparse matrix that represents a graph. Nonzero entries in matrix `G` represent the weights of the edges. `dist` are the `N` distances from the source to every node (using `Inf`s for nonreachable nodes and `0` for the source node). `path` contains the winning paths to every node. `pred` contains the predecessor nodes of the winning paths.

`[dist, path, pred] = graphshortestpath(G, S, T)` determines the single source-single destination shortest path from node `S` to node `T`.

`[...] = graphshortestpath(..., 'PropertyName', PropertyValue, ...)` calls `graphshortestpath` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[...] = graphshortestpath(..., 'Directed', DirectedValue, ...)` indicates whether the graph is directed or undirected. Set `DirectedValue` to `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.

`[...] = graphshortestpath(..., 'Method', MethodValue, ...)` lets you specify the algorithm used to find the shortest path. Choices are:

- `'Bellman-Ford'` — Assumes weights of the edges to be nonzero entries in sparse matrix `G`. Time complexity is `O(N*E)`, where `N` and `E` are the number of nodes and edges respectively.
- `'BFS'` — Breadth-first search. Assumes all weights to be equal, and nonzero entries in sparse matrix `G` to represent edges. Time

complexity is O(N+E), where N and E are the number of nodes and edges respectively.

- 'Acyclic' — Assumes G to be a directed acyclic graph and that weights of the edges are nonzero entries in sparse matrix G. Time complexity is O(N+E), where N and E are the number of nodes and edges respectively.
- 'Dijkstra' — Default algorithm. Assumes weights of the edges to be positive values in sparse matrix G. Time complexity is O(log(N)*E), where N and E are the number of nodes and edges respectively.

[...] = graphshortestpath(..., 'Weights', *WeightsValue*, ...) lets you specify custom weights for the edges. *WeightsValue* is a column vector having one entry for every nonzero value (edge) in matrix *G*. The order of the custom weights in the vector must match the order of the nonzero values in matrix *G* when it is traversed column-wise. This property lets you use zero-valued weights. By default, graphshortestpath gets weight information from the nonzero entries in matrix *G*.

Examples

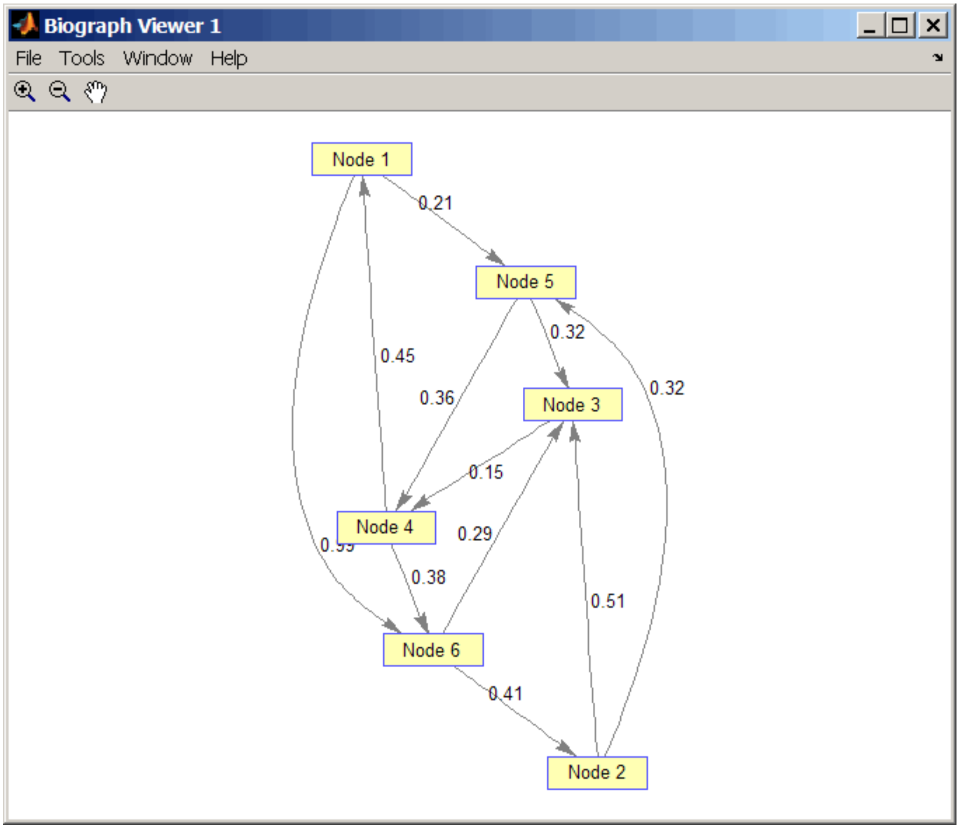
Finding the Shortest Path in a Directed Graph

1 Create and view a directed graph with 6 nodes and 11 edges.

```
W = [.41 .99 .51 .32 .15 .45 .38 .32 .36 .29 .21];
DG = sparse([6 1 2 2 3 4 4 5 5 6 1],[2 6 3 5 4 1 6 3 4 3 5],W)

DG =

   (4,1)        0.4500
   (6,2)        0.4100
   (2,3)        0.5100
   (5,3)        0.3200
   (6,3)        0.2900
   (3,4)        0.1500
   (5,4)        0.3600
   (1,5)        0.2100
```

```
(2,5)        0.3200
(1,6)        0.9900
(4,6)        0.3800
```

```
h = view(biograph(DG,[],'ShowWeights','on'))
Biograph object with 6 nodes and 11 edges.
```



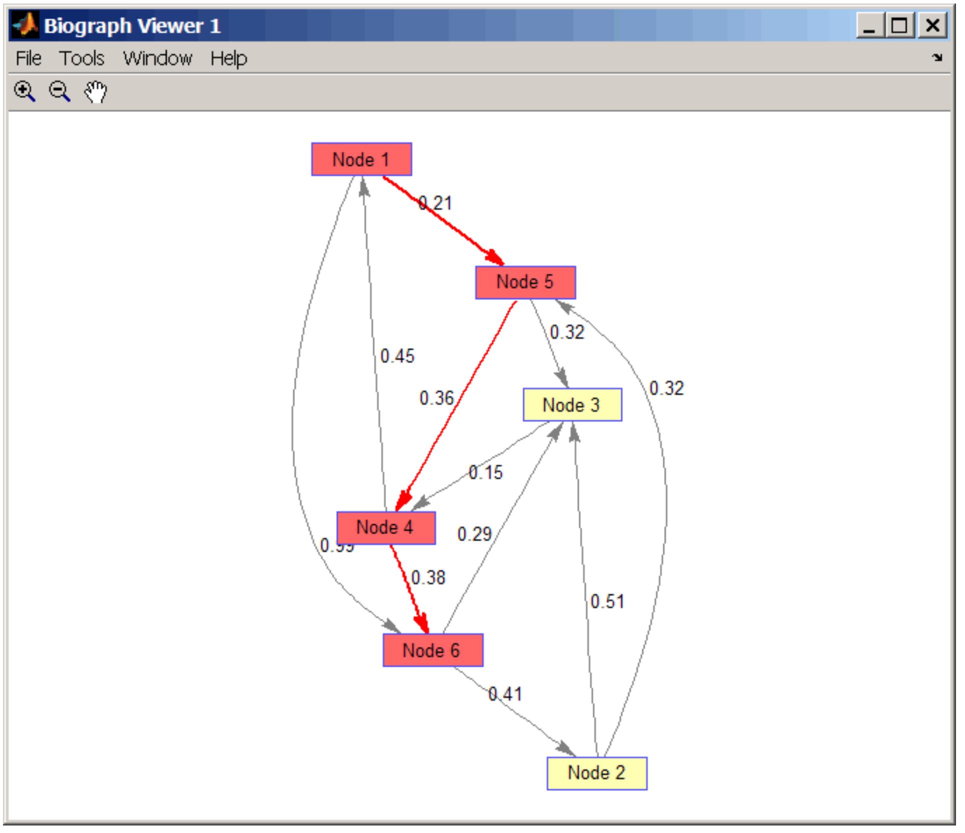
2 Find the shortest path in the graph from node 1 to node 6.

```
[dist,path,pred] = graphshortestpath(DG,1,6)
```

```
dist =

    0.9500


path =

     1     5     4     6


pred =

     0     6     5     5     1     4
```

3 Mark the nodes and edges of the shortest path by coloring them red and increasing the line width.

```
set(h.Nodes(path),'Color',[1 0.4 0.4])
edges = getedgesbynodeid(h,get(h.Nodes(path),'ID'));
set(edges,'LineColor',[1 0 0])
set(edges,'LineWidth',1.5)
```

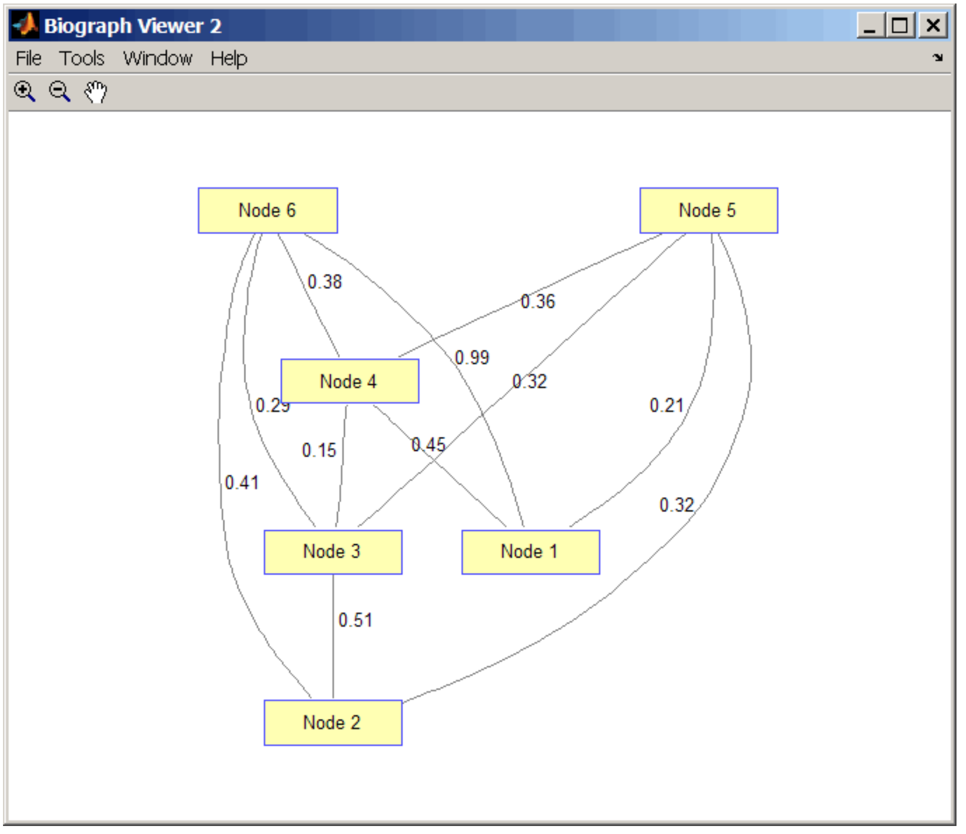


Finding the Shortest Path in an Undirected Graph

1 Create and view an undirected graph with 6 nodes and 11 edges.

```
UG = tril(DG + DG')

UG =

   (4,1)       0.4500
   (5,1)       0.2100
```

```
   (6,1)        0.9900
   (3,2)        0.5100
   (5,2)        0.3200
   (6,2)        0.4100
   (4,3)        0.1500
   (5,3)        0.3200
   (6,3)        0.2900
   (5,4)        0.3600
   (6,4)        0.3800

h = view(biograph(UG,[],'ShowArrows','off','ShowWeights','on'))
Biograph object with 6 nodes and 11 edges.
```



2 Find the shortest path in the graph from node 1 to node 6.

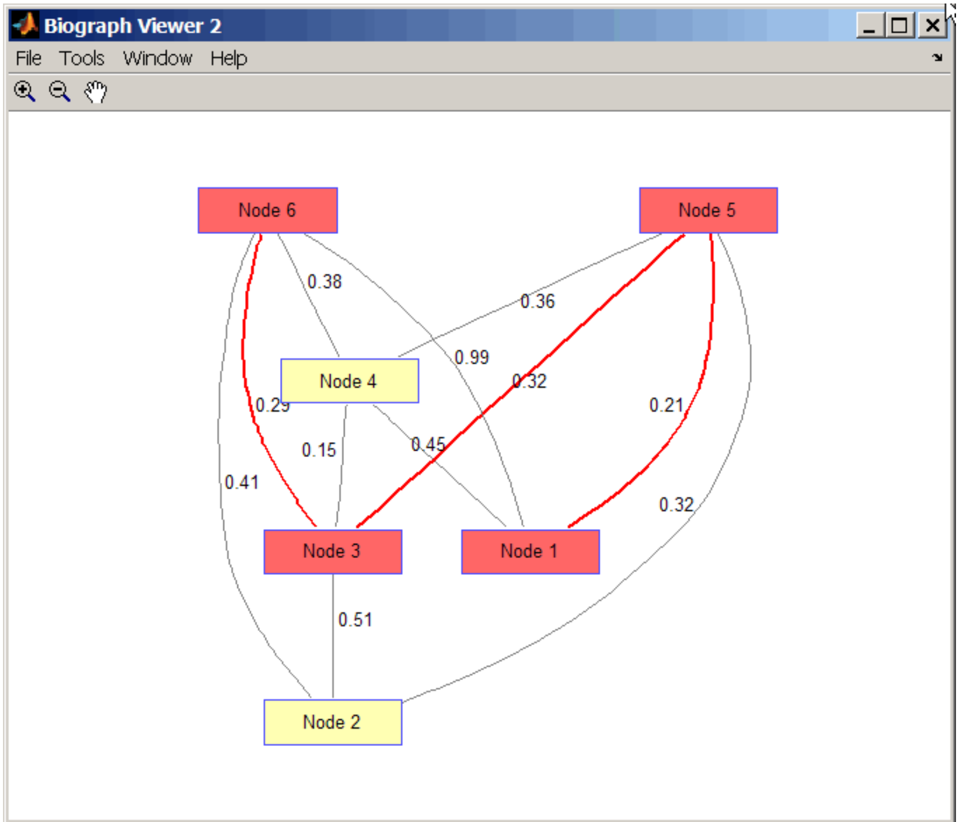
```
[dist,path,pred] = graphshortestpath(UG,1,6,'directed',false)

dist =

    0.8200


path =
```

```
     1     5     3     6


pred =

     0     5     5     1     1     3
```

3 Mark the nodes and edges of the shortest path by coloring them red and increasing the line width.

```
set(h.Nodes(path),'Color',[1 0.4 0.4])
 fowEdges = getedgesbynodeid(h,get(h.Nodes(path),'ID'));
 revEdges = getedgesbynodeid(h,get(h.Nodes(fliplr(path)),'ID'));
 edges = [fowEdges;revEdges];
 set(edges,'LineColor',[1 0 0])
 set(edges,'LineWidth',1.5)
```

graphshortestpath



References

[1] Dijkstra, E.W. (1959). A note on two problems in connexion with graphs. Numerische Mathematik *1*, 269-271.

[2] Bellman, R. (1958). On a Routing Problem. Quarterly of Applied Mathematics *16(1)*, 87-90.

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox method of `biograph object`: `shortestpath`

graphtopoorder

Purpose

Perform topological sort of directed acyclic graph

Syntax

order = graphtopoorder(*G*)

Arguments

G	N-by-N sparse matrix that represents a directed acyclic graph. Nonzero entries in matrix *G* indicate the presence of an edge.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

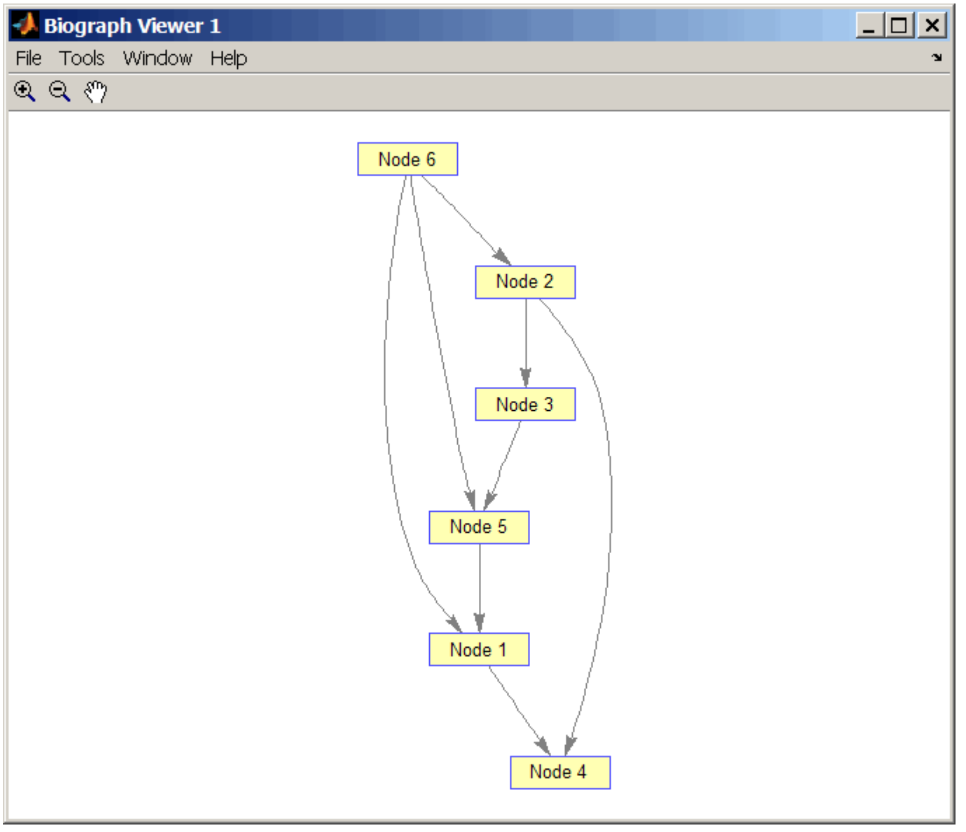
order = graphtopoorder(*G*) returns an index vector with the order of the nodes sorted topologically. In topological order, an edge can exist between a source node u and a destination node v, if and only if u appears before v in the vector *order*. *G* is an N-by-N sparse matrix that represents a directed acyclic graph (DAG). Nonzero entries in matrix *G* indicate the presence of an edge.

Examples

1 Create and view a directed acyclic graph (DAG) with six nodes and eight edges.

```
DG = sparse([6 6 6 2 2 3 5 1],[2 5 1 3 4 5 1 4],true,6,6)

DG =

   (5,1)        1
   (6,1)        1
   (6,2)        1
   (2,3)        1
   (1,4)        1
   (2,4)        1
   (3,5)        1
   (6,5)        1
```

```
view(biograph(DG))
```

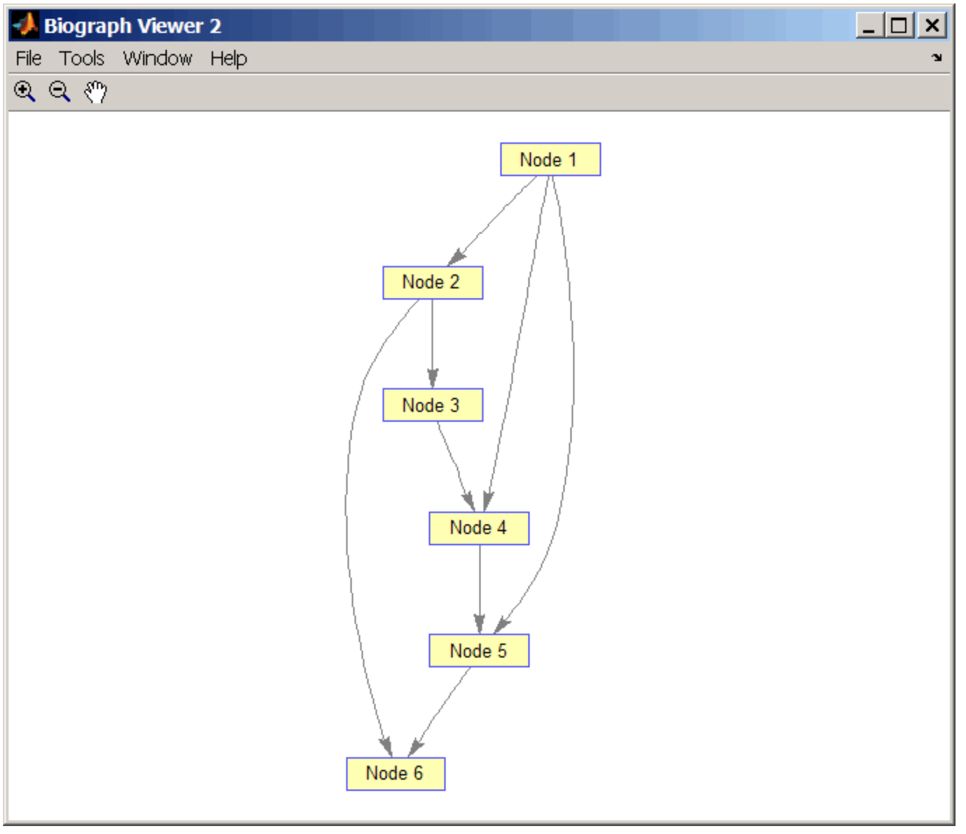


2 Find the topological order of the DAG.

```
order = graphtopoorder(DG)

order =

     6     2     3     5     1     4
```

3 Permute the nodes so that they appear ordered in the graph display.

```
DG = DG(order,order)

DG =

   (1,2)        1
   (2,3)        1
   (1,4)        1
   (3,4)        1
   (1,5)        1
   (4,5)        1
   (2,6)        1
   (5,6)        1

view(biograph(DG))
```



References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtraverse`

Bioinformatics Toolbox method of `biograph object`: `topoorder`

graphtraverse

Purpose

Traverse graph by following adjacent nodes

Syntax

```
[disc, pred, closed] = graphtraverse(G, S)
[...] = graphtraverse(G, S, ...'Depth', DepthValue, ...)
[...] = graphtraverse(G, S, ...'Directed', DirectedValue, ...)
[...] = graphtraverse(G, S, ...'Method', MethodValue, ...)
```

Arguments

G	N-by-N sparse matrix that represents a directed graph. Nonzero entries in matrix *G* indicate the presence of an edge.
S	Integer that indicates the source node in graph *G*.
DepthValue	Integer that indicates a node in graph *G* that specifies the depth of the search. Default is `Inf` (infinity).
DirectedValue	Property that indicates whether graph *G* is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.
MethodValue	String that specifies the algorithm used to traverse the graph. Choices are: • `'BFS'` — Breadth-first search. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively. • `'DFS'` — Default algorithm. Depth-first search. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

Description

Tip For introductory information on graph theory functions, see “Graph Theory Functions” in the Bioinformatics Toolbox documentation.

[*disc*, *pred*, *closed*] = graphtraverse(*G*, *S*) traverses graph G starting from the node indicated by integer S. *G* is an N-by-N sparse matrix that represents a directed graph. Nonzero entries in matrix *G* indicate the presence of an edge. *disc* is a vector of node indices in the order in which they are discovered. *pred* is a vector of predecessor node indices (listed in the order of the node indices) of the resulting spanning tree. *closed* is a vector of node indices in the order in which they are closed.

[...] = graphtraverse(*G*, *S*, ...'*PropertyName*', *PropertyValue*, ...) calls graphtraverse with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

[...] = graphtraverse(*G*, *S*, ...'Depth', *DepthValue*, ...) specifies the depth of the search. *DepthValue* is an integer indicating a node in graph *G*. Default is Inf (infinity).

[...] = graphtraverse(*G*, *S*, ...'Directed', *DirectedValue*, ...) indicates whether the graph is directed or undirected. Set *DirectedValue* to false for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is true.

[...] = graphtraverse(*G*, *S*, ...'Method', *MethodValue*, ...) lets you specify the algorithm used to traverse the graph. Choices are:

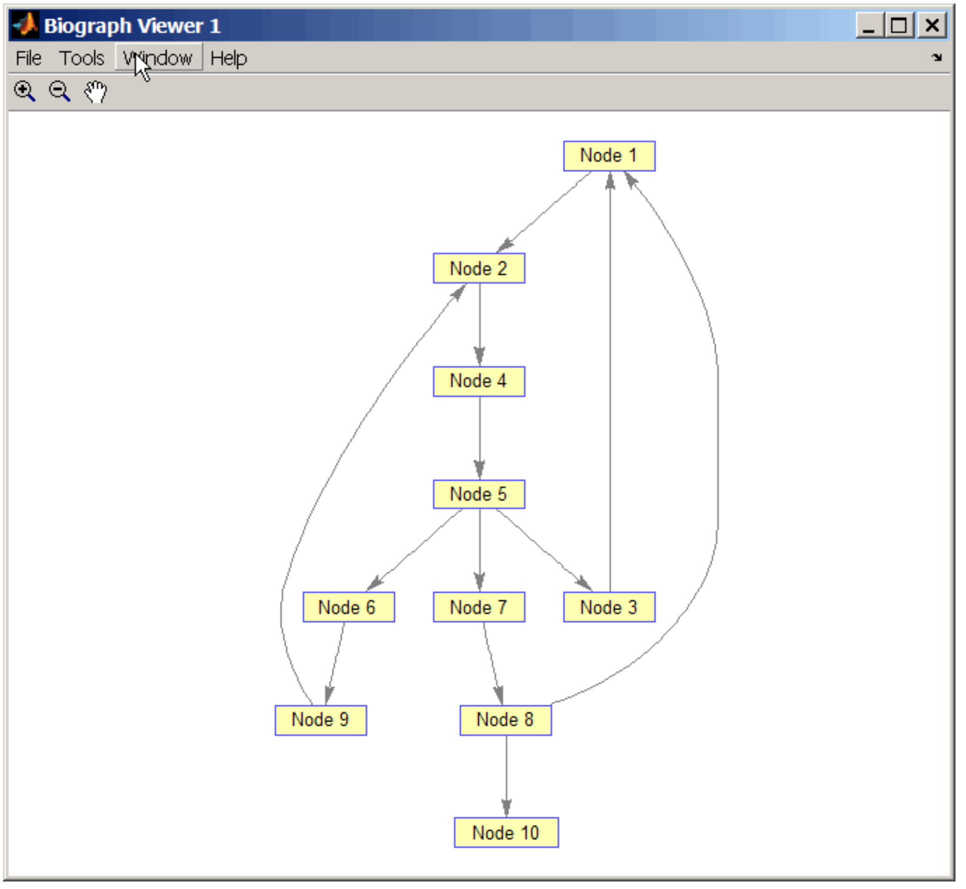
- 'BFS' — Breadth-first search. Time complexity is O(N+E), where N and E are number of nodes and edges respectively.
- 'DFS' — Default algorithm. Depth-first search. Time complexity is O(N+E), where N and E are number of nodes and edges respectively.

Examples

1 Create a directed graph with 10 nodes and 12 edges.

```
DG = sparse([1 2 3 4 5 5 5 6 7 8 8 9],...
            [2 4 1 5 3 6 7 9 8 1 10 2],true,10,10)
```

```
DG =

   (3,1)        1
   (8,1)        1
   (1,2)        1
   (9,2)        1
   (5,3)        1
   (2,4)        1
   (4,5)        1
   (5,6)        1
   (5,7)        1
   (7,8)        1
   (6,9)        1
   (8,10)       1

h = view(biograph(DG))
Biograph object with 10 nodes and 12 edges.
```

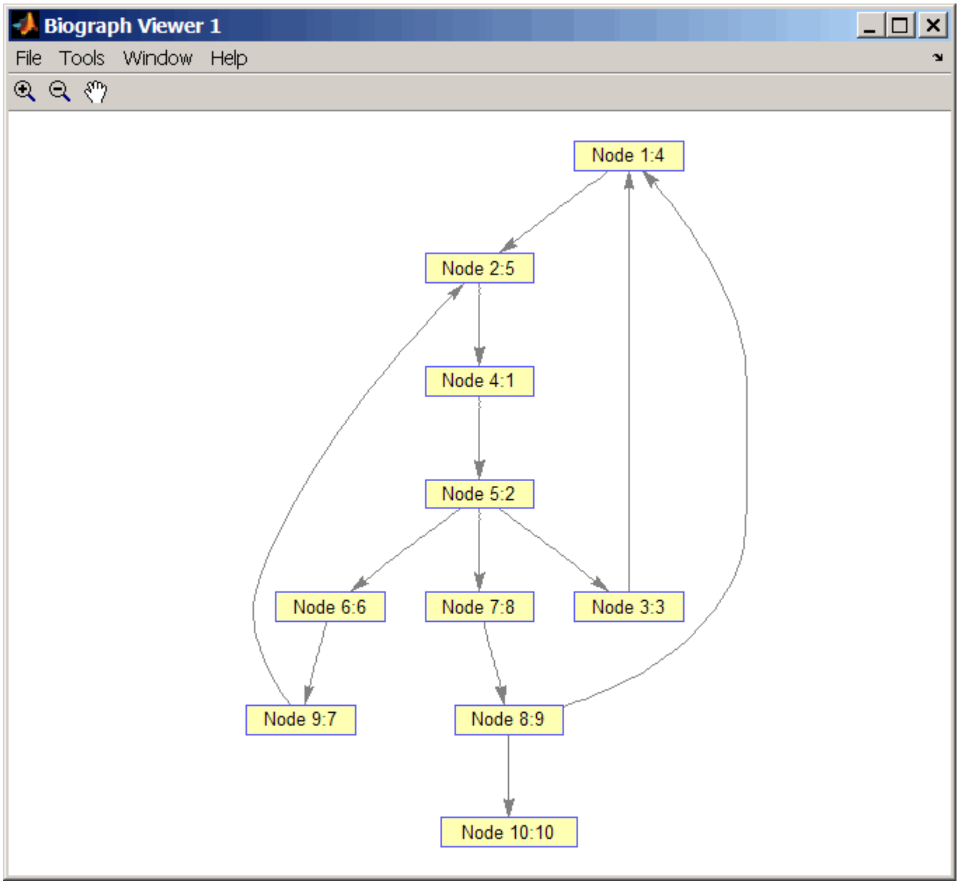


2 Traverse the graph to find the depth-first search (DFS) discovery order starting at node 4.

```
order = graphtraverse(DG,4)

order =

     4     5     3     1     2     6     9     7     8    10
```

3 Label the nodes with the DFS discovery order.

```
for i = 1:10
    h.Nodes(order(i)).Label =...
   sprintf('%s:%d',h.Nodes(order(i)).ID,i);
end
h.ShowTextInNodes = 'label'
dolayout(h)
```

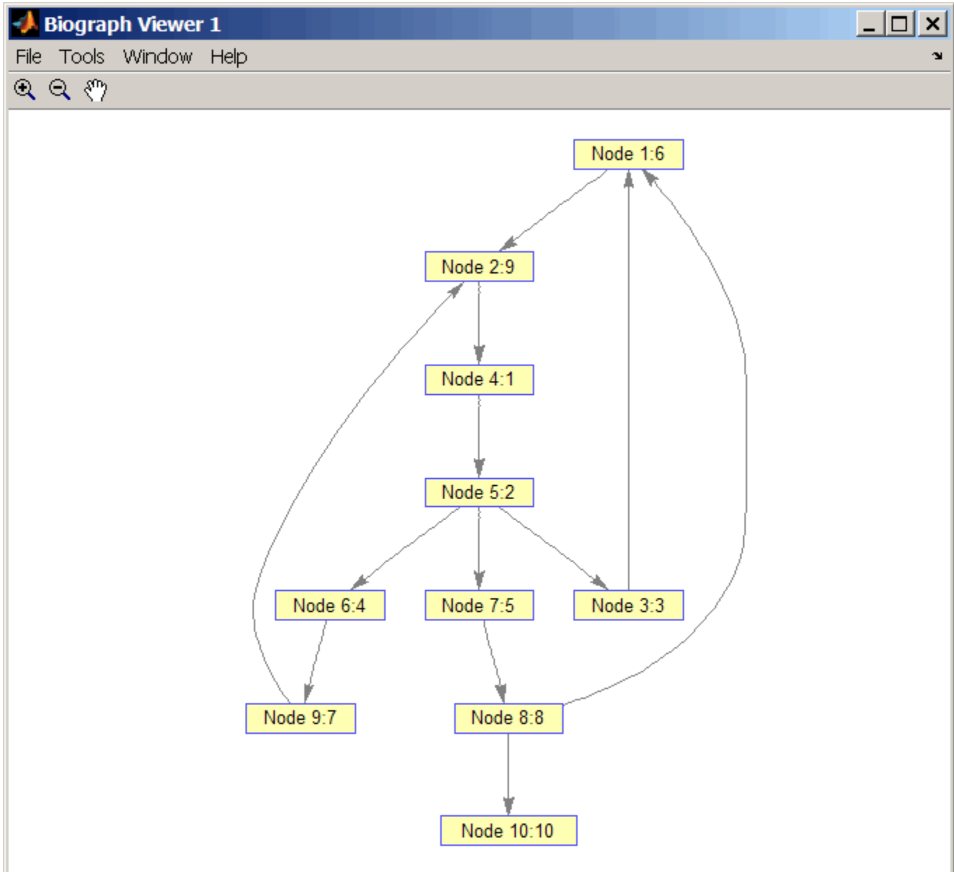


4 Traverse the graph to find the breadth-first search (BFS) discovery order starting at node 4.

```
order = graphtraverse(DG,4,'Method','BFS')

order =

     4     5     3     6     7     1     9     8     2    10
```

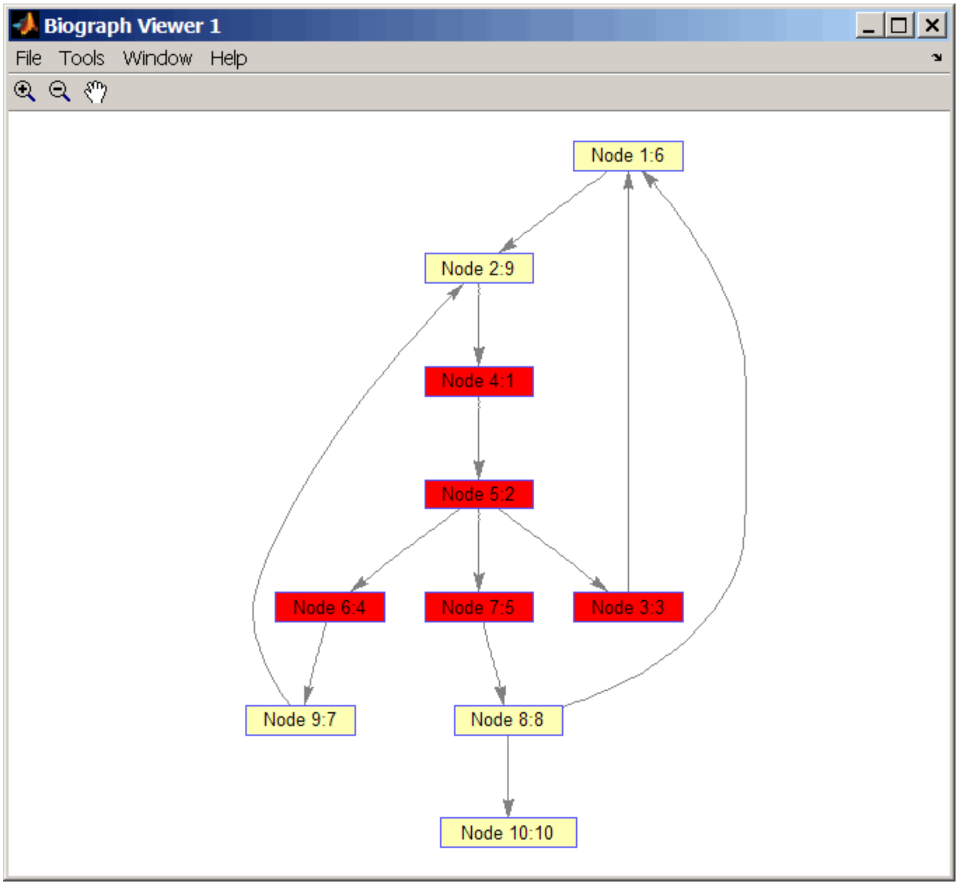
5 Label the nodes with the BFS discovery order.

```
for i = 1:10
    h.Nodes(order(i)).Label =...
   sprintf('%s:%d',h.Nodes(order(i)).ID,i);
end
h.ShowTextInNodes = 'label'
dolayout(h)
```



6 Find and color nodes that are close to (within two edges of) node 4.

```
node_idxs = graphtraverse(DG,4,'depth',2)

node_idxs =

     4     5     3     6     7

set(h.nodes(node_idxs),'Color',[1 0 0])
```



References

[1] Sedgewick, R., (2002). Algorithms in C++, Part 5 Graph Algorithms (Addison-Wesley).

[2] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`

Bioinformatics Toolbox method of `biograph object`: `traverse`

Purpose

Align query sequence to profile using hidden Markov model alignment

Syntax

```
Alignment = hmmprofalign(Model,Seq)
[Alignment, Score] = hmmprofalign(Model,Seq)
[Score, Alignment, Prointer] = hmmprofalign(Model,Seq)
hmmprofalign(..., 'PropertyName', PropertyValue,...)
hmmprofalign(..., 'ShowScore', ShowScoreValue)
hmmprofalign(..., 'Flanks', FlanksValue)
hmmprofalign(..., 'ScoreFlanks', ScoreFlanksValue)
hmmprofalign(..., 'ScoreNullTransitions',
   ScoreNullTransitionValue)
```

Arguments

Model	Hidden Markov model created with the function `hmmprofstruct`.
Seq	Amino acid or nucleotide sequence. You can also enter a structure with the field `Sequence`.
ShowScoreValue	Property to control displaying the scoring space and the winning path. Enter either `true` or `false` (default).
FlanksValue	Property to control including the symbols generated by the FLANKING INSERT states in the output sequence. Enter either `true` or `false` (default).
ScoreFlanksValue	Property to control including the transition probabilities for the flanking states in the raw score. Enter either `true` or `false` (default).
ScoreNullTransValue	Property to control adjusting the raw score using the null model for transitions (`Model.NullX`). Enter either `true` or `false` (default).

hmmprofalign

Description

Alignment = hmmprofalign(*Model,Seq*) returns the score for the optimal alignment of the query amino acid or nucleotide sequence (Seq) to the profile hidden Markov model (*Model*). Scores are computed using log-odd ratios for emission probabilities and log probabilities for state transitions.

[*Alignment, Score*] = hmmprofalign(*Model,Seq*) returns a string showing the optimal profile alignment.

Uppercase letters and dashes correspond to MATCH and DELETE states respectively (the combined count is equal to the number of states in the model). Lowercase letters are emitted by the INSERT states. For more information about the HMM profile, see hmmprofstruct.

[*Score, Alignment, Prointer*] = hmmprofalign(*Model,Seq*) returns a vector of the same length as the profile model with indices pointing to the respective symbols of the query sequence. Null pointers (NaN) mean that such states did not emit a symbol in the aligned sequence because they represent model jumps from the BEGIN state of a MATCH state, model jumps from the from a MATCH state to the END state, or because the alignment passed through DELETE states.

hmmprofalign(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

hmmprofalign(..., 'ShowScore', *ShowScoreValue*), when *ShowScoreValue* is true, displays the scoring space and the winning path.

hmmprofalign(..., 'Flanks', *FlanksValue*), when *FlanksValue* is true, includes the symbols generated by the FLANKING INSERT states in the output sequence.

hmmprofalign(..., 'ScoreFlanks', *ScoreFlanksValue*), when *ScoreFlanksValue* is true, includes the transition probabilities for the flanking states in the raw score.

hmmprofalign(..., 'ScoreNullTransitions', *ScoreNullTransitionValue*), when *ScoreNullTransitionsValue* is true, adjusts the raw score using the null model for transitions (Model.NullX).

Note Multiple target alignment is not supported in this implementation. All the `Model.LoopX` probabilities are ignored.

Examples

```
load('hmm_model_examples','model_7tm_2') % load a model example
load('hmm_model_examples','sequences')  % load a sequence example
SCCR_RABIT=sequences(2).Sequence;
[a,s]=hmmprofalign(model_7tm_2,SCCR_RABIT,'showscore',true)
```

See Also

Bioinformatics Toolbox functions `gethmmprof`, `hmmprofestimate`, `hmmprofgenerate`, `hmmprofgenerate`, `hmmprofstruct`, `pfamhmmread`, `showhmmprof`, `multialign`, `profalign`

hmmprofestimate

Purpose

Estimate profile Hidden Markov Model (HMM) parameters using pseudocounts

Syntax

```
hmmprofestimate(Model, MultipleAlignment,
                'PropertyName', PropertyValue...)

hmmprofestimate(..., 'A', AValue)
hmmprofestimate(..., 'Ax', AxValue)
hmmprofestimate(..., 'BE', BEValue)
hmmprofestimate(..., 'BDx', BDxValue)
```

Arguments

`Model`	Hidden Markov model created with the function `hmmprofstruc`.
`MultipleAlignment`	Array of sequences. `Sequences` can also be a structured array with the aligned sequences in a field `Aligned` or `Sequences`, and the optional names in a field `Header` or `Name`.
`A`	Property to set the pseudocount weight A. Default value is `20`.
`Ax`	Property to set the pseudocount weight Ax. Default value is 20.
`BE`	Property to set the background symbol emission probabilities. Default values are taken from `Model.NullEmission`.
`BMx`	Property to set the background transition probabilities from any MATCH state (`[M->M M->I M->D]`). Default values are taken from `hmmprofstruct`.
`BDx`	Property to set the background transition probabilities from any DELETE state (`[D->M D->D]`). Default values are taken from `hmmprofstruct`.

Description

`hmmprofestimate(Model, MultipleAlignment, 'PropertyName', PropertyValue...)` returns a structure with the fields containing the updated estimated parameters of a profile HMM. Symbol emission and state transition probabilities are estimated using the real counts and weighted pseudocounts obtained with the background probabilities. Default weight is `A=20`, the default background symbol emission for match and insert states is taken from `Model.NullEmission`, and the default background transition probabilities are the same as default transition probabilities returned by `hmmprofstruct`.

Model Construction: Multiple aligned sequences should contain uppercase letters and dashes indicating the model MATCH and DELETE states agreeing with `Model.ModelLength`. If model state annotation is missing, but `MultipleAlignment` is space aligned, then a "maximum entropy" criteria is used to select `Model.ModelLength` states.

Note Insert and flank insert transition probabilities are not estimated, but can be modified afterwards using `hmmprofstruct`.

`hmmprofestimate(..., 'A', AValue)` sets the pseudocount weight `A = Avalue` when estimating the symbol emission probabilities. Default value is `20`.

`hmmprofestimate(...,'Ax', AxValue)` sets the pseudocount weight `Ax = Axvalue` when estimating the transition probabilities. Default value is 20.

`hmmprofestimate(...,'BE', BEValue)` sets the background symbol emission probabilities. Default values are taken from `Model.NullEmission`.

`hmmprofestimate(...,'BMx', BMxValue)` sets the background transition probabilities from any MATCH state (`[M->M M->I M->D]`). Default values are taken from `hmmprofstruct`.

`hmmprofestimate(..., 'BDx', BDxValue)` sets the background transition probabilities from any DELETE state (`[D->M D->D]`). Default values are taken from `hmmprofstruct`.

See Also

Bioinformatics Toolbox functions `hmmprofalign`, `hmmprofstruct`, `showhmmprof`

Purpose

Generate random sequence drawn from profile Hidden Markov Model (HMM)

Syntax

```
Sequence = hmmprofgenerate(Model)
[Sequence, Profptr] = hmmprofgenerate(Model)
... = hmmprofgenerate(Model, ...'Align', AlignValue, ...)
... = hmmprofgenerate(Model, ...'Flanks', FlanksValue, ...)
... = hmmprofgenerate(Model, ...'Signature', SignatureValue,
    ...)
```

Arguments

Model	Hidden Markov model created with the `hmmprofstruct` function.
AlignValue	Property to control using uppercase letters for matches and lowercase letters for inserted letters. Enter either `true` or `false`. Default is `false`.
FlanksValue	Property to control including the symbols generated by the FLANKING INSERT states in the output sequence. Enter either `true` or `false`. Default is `false`.
SignatureValue	Property to control returning the most likely path and symbols. Enter either `true` or `false`. Default is `false`.

Description

`Sequence = hmmprofgenerate(Model)` returns the string *Sequence* showing a sequence of amino acids or nucleotides drawn from the profile *Model*. The length, alphabet, and probabilities of the *Model* are stored in a structure. For move information about this structure, see `hmmprofstruct`.

`[Sequence, Profptr] = hmmprofgenerate(Model)` returns a vector of the same length as the profile model pointing to the respective states in the output sequence. Null pointers (0) mean that such states do not exist in the output sequence, either because they are never touched (i.e., jumps from the BEGIN state to MATCH states or from MATCH states to the END state), or because DELETE states are not in the output sequence (not aligned output; see below).

`... = hmmprofgenerate(Model, ...'PropertyName', PropertyValue, ...)` calls `hmmprofgenerate` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`... = hmmprofgenerate(Model, ...'Align', AlignValue, ...)` if `Align` is `true`, the output sequence is aligned to the model as follows: uppercase letters and dashes correspond to MATCH and DELETE states respectively (the combined count is equal to the number of states in the model). Lowercase letters are emitted by the INSERT or FLANKING INSERT states. If *`AlignValue`* is `false`, the output is a sequence of uppercase symbols. The default value is `true`.

`... = hmmprofgenerate(Model, ...'Flanks', FlanksValue, ...)` if `Flanks` is `true`, the output sequence includes the symbols generated by the FLANKING INSERT states. The default value is `false`.

`... = hmmprofgenerate(Model, ...'Signature', SignatureValue, ...)` if *`SignatureValue`* is `true`, returns the most likely path and symbols. The default value is `false`.

Examples

```
load('hmm_model_examples','model_7tm_2') % load a model example
rand_sequence = hmmprofgenerate(model_7tm_2)
```

See Also

Bioinformatics Toolbox functions: `hmmprofalign`, `hmmprofstruct`, `showhmmprof`

Purpose

Concatenate prealigned strings of several sequences to profile Hidden Markow Model (HMM)

Syntax

```
hmmprofmerge(Sequences)
hmmprofmerge(Sequences, Names)
hmmprofmerge(Sequences, Names, Scores)
```

Arguments

Sequences	Array of sequences. *Sequences* can also be a structured array with the aligned sequences in a field `Aligned` or `Sequences`, and the optional names in a field `Header` or `Name`.
Names	Names for the sequences. Enter a vector of names.
Scores	Pairwise alignment scores from the function hmmprofalign. Enter a vector of values with the same length as the number of sequences in *Sequences*.

Description

`hmmprofmerge(`*Sequences*`)` displays a set of prealigned `sequences` to a HMM model profile. The output is aligned corresponding to the HMM states.

- Match states — Uppercase letters
- Insert states — Lowercase letters or asterisks (*)
- Delete states — Dashes

Periods (.) are added at positions corresponding to inserts in other sequences. The input sequences must have the same number of profile states, that is, the joint count of capital letters and dashes must be the same.

`hmmprofmerge(`*Sequences*`, `*Names*`)` labels the sequences with `Names`.

`hmmprofmerge(`*Sequences*`, `*Names*`, `*Scores*`)` sorts the displayed sequences using `Scores`.

Examples

```
load('hmm_model_examples','model_7tm_2')  %load model
load('hmm_model_examples','sequences')  %load sequences

for ind =1:length(sequences)
    [scores(ind),sequences(ind).Aligned] =...
        hmmprofalign(model_7tm_2,sequences(ind).Sequence);
    end
hmmprofmerge(sequences, scores)
```

See Also

Bioinformatics Toolbox functions: `hmmprofalign`, `hmmprofstruct`

Purpose

Create profile Hidden Markov Model (HMM) structure

Syntax

```
Model = hmmprofstruct(Length)
Model = hmmprofstruct(Length, 'Field1', FieldValues1,...)
hmmprofstruct(Model, 'Field1', Field1Values1,...)
```

Arguments

`Length`	Number of match states in the model.
`Model`	Hidden Markov model created with the function `hmmprofstruct`.
`Field1`	Field name in the structure `Model`. Enter a name from the table below.

Description

`Model = hmmprofstruct(Length)` returns a structure with the fields containing the required parameters of a profile HMM. `Length` specifies the number of match states in the model. All other mandatory model parameters are initialized to the default values.

`Model = hmmprofstruct(Length, 'Field1',` *`FieldValues1`*`, ...)` creates a profile HMM using the specified fields and parameters. All other mandatory model parameters are initialized to default values.

`hmmprofstruct(Model, 'Field1',` *`Field1Values1`*`, ...)` returns the updated profile HMM with the specified fields and parameters. All other mandatory model parameters are taken from the reference MODEL.

HMM Profile Structure Format

Model parameters fields (mandatory). All probability values are in the [0 1] range.

Field Name	Description
`ModelLength`	Length of the profile (number of MATCH states)
`Alphabet`	`'AA'` or `'NT'`. Default is `'AA'`.

Field Name	Description
MatchEmission	Symbol emission probabilities in the MATCH states. Size is [ModelLength x AlphaLength]. Defaults to uniform distributions. May accept a structure with residue counts (see aacount or basecount).
InsertEmission	Symbol emission probabilities in the INSERT state. Size is [ModelLength x AlphaLength]. Defaults to uniform distributions. May accept a structure with residue counts (see aacount or basecount).
NullEmission	Symbol emission probabilities in the MATCH and INSERT states for the NULL model. NULL model, size is [1 x AlphaLength]. Defaults to a uniform distribution. May accept a structure with residue counts (see aacount or basecount). The NULL model is used to compute the log-odds ratio at every state and avoid overflow when propagating the probabilities through the model.

BeginX	BEGIN state transition probabilities.
	
	Format is
	
	`[B->D1 B->M1 B->M2 B->M3 .... B->Mend]`
	
	Notes:
	
	`sum(S.BeginX) = 1`
	
	For fragment profiles
	
	`sum(S.BeginX(3:end)) = 0`
	
	Default is [0.01 0.99 0 0 ... 0].

<table>
<tr><th>Field Name</th><th>Description</th></tr>
<tr><td><code>MatchX</code></td><td>MATCH state transition probabilities
Format is
<pre>[M1->M2 M2->M3 ... M[end-1]->Mend;
M1->I1 M2->I2 ... M[end-1]->I[end-1];
M1->D2 M2->D3 ... M[end-1]->Dend;
M1->E M2->E ... M[end-1]->E]</pre>Notes:
<pre>sum(S.MatchX) = [1 1 ... 1]</pre>For fragment profiles
<pre>sum(S.MatchX(4,:)) = 0</pre>Default is <code>repmat([0.998 0.001 0.001 0],profLength-1,1)</code>.</td></tr>
<tr><td><code>InsertX</code></td><td>INSERT state transition probabilities
Format is
<pre>[I1->M2 I2->M3 ... I[end-1]->Mend;
[I1->I1 I2->I2 ... I[end-1]->I[end-1]]</pre>Note:
<pre>sum(S.InsertX) = [1 1 ... 1]</pre>Default is <code>repmat([0.5 0.5],profLength-1,1)</code>.</td></tr>
</table>

Field Name	Description

`DeleteX`	DELETE state transition probabilities. The format is
	`[D1->M2 D2->M3 ... D[end-1]->Mend ;`
	`[D1->D2 D2->D3 ... D[end-1]->Dend  ]`
	Note `sum(S.DeleteX) = [ 1 1 ...  1 ]`
	Default is `repmat([0.5 0.5],profLength-1,1)`.

`FlankingInsertX`	Flanking insert states (N and C) used for LOCAL profile alignment. The format is
	`[N->B  C->T ;`
	`[N->N  C->C ]`
	Note `sum(S.FlankingInsertsX) = [1 1]`
	To force global alignment use
	`S.FlankingInsertsX = [1 1; 0 0]`
	Default is `[0.01 0.01; 0.99 0.99]`.

Field Name	Description

LoopX	Loop states transition probabilities used for multiple hits alignment. The format is
	
	`[E->C  J->B ;`
	`E->J  J->J ]`
	
	Note `sum(S.LoopX) = [1 1]`
	
	Default is `[0.5 0.01; 0.5 0.99]`

NullX	Null transition probabilities used to provide scores with log-odds values also for state transitions. The format is `[G->F ; G->G]` **Note** `sum(S.NullX) = 1` Default is `[0.01; 0.99]`

Annotation Fields (Optional)

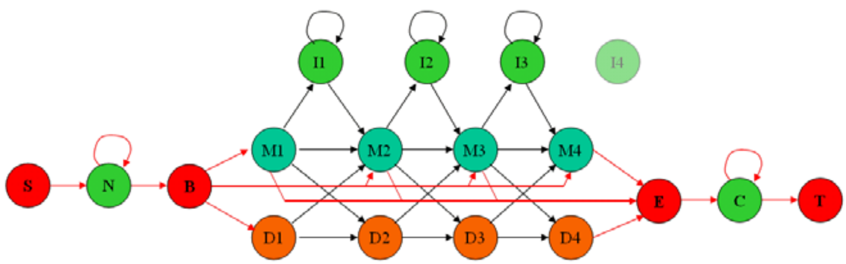
Name	Model Name
IDNumber	Identification Number
Description	Short description of the model

A profile Markov model is a common statistical tool for modeling structured sequences composed of symbols . These symbols include randomness in both the output (emission of symbols) and the state transitions of the process. Markov models are generally represented by state diagrams.

The figure shown below is a state diagram for a HMM profile of length 4. Insert, match, and delete states are in the regular part (middle section).

- Match state means that the target sequence is aligned to the profile at the specific location.
- Delete state represents a gap or symbol absence in the target sequence (also know as a silent state because it does not emit any symbol).
- Insert state represents the excess of one or more symbols in the target sequence that are not included in the profile.

Flanking states (`S`, `N`, `B`, `E`, `C`, `T`) are used for proper modeling of the ends of the sequence, either for global, local or fragment alignment of the profile. `S`, `N`, `E`, and `T` are silent while `N` and `C` are used to insert symbols at the flanks.



Examples

```
hmmprofstruct(100,'Alphabet','AA')
```

See Also

Bioinformatics Toolbox functions: `aacount`, `basecount`, `gethmmprof`, `hmmprofalign`, `hmmprofestimate`, `hmmprofgenerate`, `hmmprofmerge`, `pfamhmmread`, `showhmmprof`

Purpose

Read microarray data from ImaGene Results file

Syntax

```
imagenedata = imageneread('File')
imagenedata = imageneread(..., 'CleanColNames',
CleanColNamesValue, ...)
```

Arguments

File	ImaGene Results formatted file. Enter a file name or a path and file name.
CleanColNameValue	Property to control creating column names that MATLAB can use as variable names.

Description

`imagenedata = imageneread('File')` reads ImaGene results data from *File* and creates a MATLAB structure `imagedata` containing the following fields:

Field
HeaderAA
Data
Blocks
Rows
Columns
Fields
IDs
ColumnNames

Field
Indices
Shape

imagenedata = imageneread(..., '*PropertyName*', *PropertyValue*, ...) defines optional properties using property name/value pairs, described as follows:

imagenedata = imageneread(..., 'CleanColNames', *CleanColNamesValue*, ...). An ImaGene file may contain column names with spaces and some characters that MATLAB cannot use in MATLAB variable names. If *CleanColNamesValue* is true, imagene returns, in the field ColumnNames, names that are valid MATLAB variable names and names that you can use in functions. By default, *CleanColNamesValue* is false and the field ColumnNames may contain characters that are not valid for MATLAB variable names.

The field Indices of the structure contains MATLAB indices that you can use for plotting heat maps of the data with the function image or imagesc.

For more details on the ImaGene format and example data, see the ImaGene User Manual.

ImaGene is a registered trademark of BioDiscovery, Inc.

Examples

1 Read in a sample ImaGene Results file. Note, the file cy3.txt is not provided with Bioinformatics Toolbox.

```
cy3Data = imageneread('cy3.txt');
```

2 Plot the signal mean.

```
maimage(cy3Data,'Signal Mean');
```

3 Read in a sample ImaGene Results file. Note, the file cy5.txt is not provided with Bioinformatics Toolbox.

```
cy5Data = imageneread('cy5.txt');
```

4 Create a loglog plot of the signal median from two ImaGene Results files.

```
sigMedianCol = find(strcmp('Signal Median',cy3Data.ColumnNames));
cy3Median = cy3Data.Data(:,sigMedianCol);
cy5Median = cy5Data.Data(:,sigMedianCol);
maloglog(cy3Median,cy5Median,'title','Signal Median');
```

See Also

Bioinformatics Toolbox functions: `gprread`, `maboxplot`, `maimage`, `sptread`

Purpose

Convert amino acid sequence from integer to letter representation

Syntax

```
SeqChar = int2aa(SeqInt)
SeqChar = int2aa(SeqInt, 'Case', CaseValue)
```

Arguments

SeqInt	Row vector of integers specifying an amino acid sequence. See the table Mapping Amino Acid Integers to Letters on page 2-326 for valid integers. Integers are arbitrarily assigned to IUB/IUPAC letters.
CaseValue	String that specifies the case of the returned character string. Choices are `'upper'` (default) or `'lower'`.

Return Values

SeqChar	Character string of single-letter codes specifying an amino acid sequence.

Mapping Amino Acid Integers to Letters

Amino Acid	Integer	Code
Alanine	1	A
Arginine	2	R
Asparagine	3	N
Aspartic acid (Aspartate)	4	D
Cysteine	5	C
Glutamine	6	Q
Glutamic acid (Glutamate)	7	E
Glycine	8	G

Amino Acid	Integer	Code
Histidine	9	H
Isoleucine	10	I
Leucine	11	L
Lysine	12	K
Methionine	13	M
Phenylalanine	14	F
Proline	15	P
Serine	16	S
Threonine	17	T
Tryptophan	18	W
Tyrosine	19	Y
Valine	20	V
Aspartic acid or Asparagine	21	B
Glutamic acid or glutamine	22	Z
Any amino acid	23	X
Translation stop	24	*
Gap of indeterminate length	25	-
Unknown or any integer not in table	0	?

Description

`SeqChar = int2aa(SeqInt)` converts a 1-by-N array of integers specifying an amino acid sequence to a character string of single-letter codes specifying the same amino acid sequence. See the table Mapping Amino Acid Integers to Letters on page 2-326 for valid integers.

`SeqChar = int2aa(SeqInt, 'Case', CaseValue)` specifies the case of the returned character string representing an amino acid sequence. Choices are `'upper'` (default) or `'lower'`.

Examples

Convert an amino acid sequence from integer to letter representation.

```
s = int2aa([13 1 17 11 1 21])

s =

MATLAB
```

See Also

Bioinformatics Toolbox functions: `aa2int`, `aminolookup`, `int2nt`, `nt2int`

Purpose

Convert nucleotide sequence from integer to letter representation

Syntax

```
int2nt(SeqNT)
int2nt(..., 'PropertyName', PropertyValue,...)
int2nt(..., 'Alphabet', AlphabetValue)
int2nt(..., 'Unknown', UnknownValue)
int2nt(..., 'Case', CaseValue)
```

Arguments

SeqNT	Nucleotide sequence represented by integers. Enter a vector of integers from the table Mapping Nucleotide Integers to Letters below. The array does not have to be of type integer, but it does have to contain only integer numbers. Integers are arbitrarily assigned to IUB/IUPAC letters.
AlphabetValue	Property to select the nucleotide alphabet. Enter either `'DNA'` or `'RNA'`.
UnknownValue	Property to select the integer value for the unknown character. Enter a character to map integers `16` or greater to an unknown character. The character must not be one of the nucleotide characters `A`, `T`, `C`, `G` or the ambiguous nucleotide characters `N`, `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, or `V`. The default character is `*`.
CaseValue	Property to select the letter case for the nucleotide sequence. Enter either `'upper'` (default) or `'lower'` .

Mapping Nucleotide Integers to Letters

Base	Code	Base	Code	Base	Code
Adenosine	1—A	T, C (pyrimidine)	6—Y	A, T, G (not C)	12—D
Cytidine	2—C	G, T (keto)	7—K	A, T, C (not G)	13—H
Guanine	3—G	A, C (amino)	8—M	A, G, C (not T)	14—V
Thymidine	4—T	G, C (strong)	9—S	A, T, G, C (any)	15—N
Uridine (if 'Alphabet' = 'RNA'	4—U	A, T (weak)	10—W	Gap of indeterminate length	16 — -
A, G (purine)	5—R	T, G, C (not A)	11—B	Unknown (default)	0 and ≥17—*

Description

`int2nt(`*`SeqNT`*`)` converts a 1-by-N array of integers to a character string using the table Mapping Nucleotide Letters to Integers above.

`int2nt(..., '`*`PropertyName`*`', `*`PropertyValue`*`,...)` defines optional properties using property name/value pairs.

`int2nt(..., 'Alphabet', `*`AlphabetValue`*`)` selects the nucleotide alphabet to use. The default value is `'DNA'`, which uses the symbols `A`, `T`, `C`, and `G`. If *`AlphabetValue`* is set to `'RNA'`, `int2nt` uses the symbols `A`, `C`, `U`, `G` instead.

`int2nt(..., 'Unknown', `*`UnknownValue`*`)` specifies the character to represent an unknown nucleotide base.

`int2nt(..., 'Case', `*`CaseValue`*`)` selects the output case of the nucleotide string.

Examples

Enter a sequence of integers as a MATLAB vector (space or comma-separated list with square brackets).

```
s = int2nt([1 2 4 3 2 4 1 3 2])

s =
   ACTGCTAGC
```

Define a symbol for unknown numbers 16 and greater.

```
si = [1 2 4 20 2 4 40 3 2];
s = int2nt(si, 'unknown', '#')

s =
ACT#CT#GC
```

See Also

Bioinformatics Toolbox function `aa2int`, `int2aa`, `nt2int`

isoelectric

Purpose

Estimate isoelectric point for amino acid sequence

Syntax

```
pI = isoelectric(SeqAA)
[pI Charge] = isoelectric(SeqAA)
isoelectric(..., 'PropertyName', PropertyValue,...)
isoelectric(..., 'PKVals', PKValsValue)
isoelectric(..., 'Charge', ChargeValue)
isoelectric(..., 'Chart', ChartValue)
```

Arguments

SeqAA	Amino acid sequence. Enter a character string or a vector of integers from the table. Examples: `'ARN'` or `[1 2 3]`.
PKValsValue	Property to provide alternative pK values.
ChargeValue	Property to select a specific pH for estimating charge. Enter a number between `0` and `14`. The default value is `7.2`.
ChartValue	Property to control plotting a graph of charge versus pH. Enter `true` or `false`.

Description

`pI = isoelectric(SeqAA)` returns the estimated isoelectric point (*pI*) for an amino acid sequence. The isoelectric point is the pH at which the protein has a net charge of zero

`[pI Charge] = isoelectric(SeqAA)` returns the estimated isoelectric point (*pI*) for an amino acid sequence and the estimated charge for a given pH (default is typical intracellular pH `7.2`).

The estimates are skewed by the underlying assumptions that all amino acids are fully exposed to the solvent, that neighboring peptides have no influence on the pK of any given amino acid, and that the constitutive amino acids, as well as the N- and C-termini, are unmodified. Cysteine residues participating in disulfide bridges also affect the true pI and are not considered here. By default, `isoelectric` uses the EMBOSS amino acid pK table, or you can substitute other values using the property `PKVals`.

- If the sequence contains ambiguous amino acid characters (b z * –), `isoelectric` ignores the characters and displays a warning message.

  ```
  Warning: Symbols other than the standard 20 amino acids
  appear in the sequence.
  ```

- If the sequence contains undefined amino acid characters (`i j o`), `isoelectric` ignores the characters and displays a warning message.

  ```
  Warning: Sequence contains unknown characters. These will
  be ignored.
  ```

`isoelectric(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`isoelectric(..., 'PKVals', PKValsValue)` uses the alternative pK table stored in the text file *`PKValValues`*. For an example of a pK text file, see the file `Emboss.pK`.

```
N_term 8.6
K 10.8
R 12.5
H 6.5
D 3.9
E 4.1
C 8.5
Y 10.1
C_term 3.6
```

`isoelectric(..., 'Charge', ChargeValue)` returns the estimated charge of a sequence for a given pH (*`ChargeValue`*).

`isoelectric(..., 'Chart', ChartValue)` when *ChartValue* is `true`, returns a graph plotting the charge of the protein versus the pH of the solvent.

Example

```
% Get a sequence from PDB.
pdbSeq = getpdb('1CIV', 'SequenceOnly', true)
% Estimate its isoelectric point.
isoelectric(pdbSeq)

% Plot the charge against the pH for a short polypeptide sequence.
isoelectric('PQGGGGWGQPHGGGWGQPHGGGGWGQGGSHSQG', 'CHART', true)

% Get the Rh blood group D antigen from NCBI and calculate
% its charge at pH 7.3 (typical blood pH).
gpSeq = getgenpept('AAB39602')
[pI Charge] = isoelectric(gpSeq, 'Charge', 7.38)
```

See Also

Bioinformatics functions `aacount`, `molweight`

Purpose

Read JCAMP-DX formatted files

Syntax

`JCAMPData = jcampread(File)`

Arguments

File	JCAMP-DX formatted file (ASCII text file). Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text of a JCAMP-DX formatted file.

Description

JCAMP-DX is a file format for infrared, NMR, and mass spectrometry data from the Joint Committee on Atomic and Molecular Physical Data (JCAMP). `jcampread` supports reading data from files saved with Versions `4.24` and `5` of the JCAMP-DX format. For more details, see

```
http://www.jcamp.org/index.html
```

`JCAMPData` = `jcampread(`*`File`*`)`reads data from a JCAMP-DX formatted file (*`File`*) and creates a MATLAB structure (*`JCAMPData`*) containing the following fields:

Field
`Title`
`DataType`
`Origin`
`Owner`
`Blocks`
`Notes`

The `Blocks` field of the structure is an array of structures corresponding to each set of data in the file. These structures have the following fields:

Field
XData
YData
XUnits
YUnits
Notes

Examples

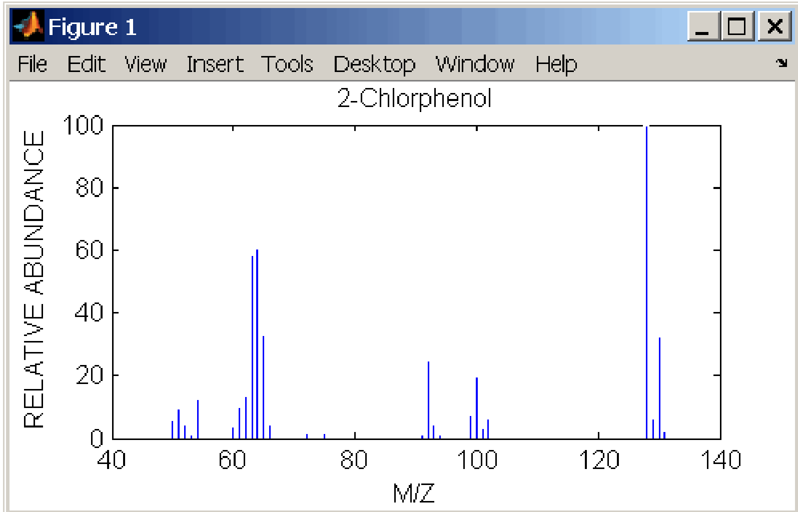
1 Download test data in the file isa_ms1.dx from

```
http://www.jcamp.org/testdata.html/testdata.zip
```

2 Read a JCAMP-DX file (isas_ms1.dx) into MATLAB and plot the mass spectrum.

```
jcampStruct = jcampread('isas_ms1.dx')
data = jcampStruct.Blocks(1);
stem(data.XData,data.YData, '.', 'MarkerEdgeColor','w');
title(jcampStruct.Title);
xlabel(data.XUnits);
ylabel(data.YUnits);
```

A figure window opens with the mass spectrum.



See Also

Bioinformatics Toolbox functions: `mslowess`, `mssgolay`, `msviewer`, `mzxmlread`

joinseq

Purpose

Join two sequences to produce shortest supersequence

Syntax

`SeqNT3 = joinseq(SeqNT1, SeqNT2)`

Arguments

SeqNT1, *SeqNT2*	Nucleotide sequences.

Description

`SeqNT3 = joinseq(SeqNT1, SeqNT2)` creates a new sequence that is the shortest supersequence of *SeqNT1* and *SeqNT2*. If there is no overlap between the sequences, then *SeqNT2* is concatenated to the end of *SeqNT1*. If the length of the overlap is the same at both ends of the sequence, then the overlap at the end of *SeqNT1* and the start of *SeqNT2* is used to join the sequences.

If *SeqNT1* is a subsequence of *SeqNT2*, then *SeqNT2* is returned as the shortest supersequence and vice versa.

Examples

```
seq1 = 'ACGTAAA';
seq2 = 'AAATGCA';
joined = joinseq(seq1,seq2)

joined =
    ACGTAAATGCA
```

See Also

MATLAB functions `cat`, `strcat`, `strfind`

Purpose

Classify data using nearest neighbor method

Syntax

```
Class = knnclassify(Sample, Training, Group)
Class = knnclassify(Sample, Training, Group, k)
Class = knnclassify(Sample, Training, Group, k, distance)
Class = knnclassify(Sample, Training, Group, k, distance,
    rule)
```

Arguments

Sample	Matrix whose rows will be classified into groups. *Sample* must have the same number of columns as *Training*.
Training	Matrix used to group the rows in the matrix *Sample*. *Training* must have the same number of columns as *Sample*. Each row of *Training* belongs to the group whose value is the corresponding entry of *Group*.
Group	Vector whose distinct values define the grouping of the rows in *Training*.
k	The number of nearest neighbors used in the classification. Default is 1.

distance	String to specify the distance metric. Choices are: • `'euclidean'` — Euclidean distance (default) • `'cityblock'` — Sum of absolute differences • `'cosine'` — One minus the cosine of the included angle between points (treated as vectors) • `'correlation'` — One minus the sample correlation between points (treated as sequences of values) • `'hamming'` — Percentage of bits that differ (only suitable for binary data)
rule	String to specify the rule used to decide how to classify the sample. Choices are: • `'nearest'` — Majority rule with nearest point tie-break (default) • `'random'` — Majority rule with random point tie-break • `'consensus'` — Consensus rule

Description

`Class = knnclassify(Sample, Training, Group)` classifies the rows of the data matrix *Sample* into groups, based on the grouping of the rows of *Training*. *Sample* and *Training* must be matrices with the same number of columns. *Group* is a vector whose distinct values define the grouping of the rows in *Training*. Each row of *Training* belongs to the group whose value is the corresponding entry of *Group*. `knnclassify` assigns each row of `Sample` to the group for the closest row of *Training*. *Group* can be a numeric vector, a string array, or a cell array of strings. *Training* and *Group* must have the same number of rows. `knnclassify` treats `NaN`s or empty strings in *Group* as missing values, and ignores the corresponding rows of *Training*. *Class* indicates which group each row of *Sample* has been assigned to, and is of the same type as *Group*.

`Class = knnclassify(Sample, Training, Group, k)` enables you to specify `k`, the number of nearest neighbors used in the classification. Default is `1`.

Class = knnclassify(*Sample*, *Training*, *Group*, *k*, *distance*) enables you to specify the distance metric. Choices for *distance* are:

'euclidean'	Euclidean distance (default)
'cityblock'	Sum of absolute differences
'cosine'	One minus the cosine of the included angle between points (treated as vectors)
'correlation'	One minus the sample correlation between points (treated as sequences of values)
'hamming'	Percentage of bits that differ (only suitable for binary data)

Class = knnclassify(*Sample*, *Training*, *Group*, *k*, *distance*, *rule*) enables you to specify the rule used to decide how to classify the sample. Choices for *rule* are:

'nearest'	Majority rule with nearest point tie-break (default)
'random'	Majority rule with random point tie-break
'consensus'	Consensus rule

The default behavior is to use majority rule. That is, a sample point is assigned to the class the majority of the k nearest neighbors are from. Use 'consensus' to require a consensus, as opposed to majority rule. When using the 'consensus' option, points where not all of the k nearest neighbors are from the same class are not assigned to one of the classes. Instead the output Class for these points is NaN for numerical groups or '' for string named groups. When classifying to more than two groups or when using an even value for k, it might be necessary to break a tie in the number of nearest neighbors. Options are 'random', which selects a random tiebreaker, and 'nearest', which uses the nearest neighbor among the tied groups to break the tie. The default behavior is majority rule, with nearest tie-break.

Examples

Classifying Rows

The following example classifies the rows of the matrix `sample`:

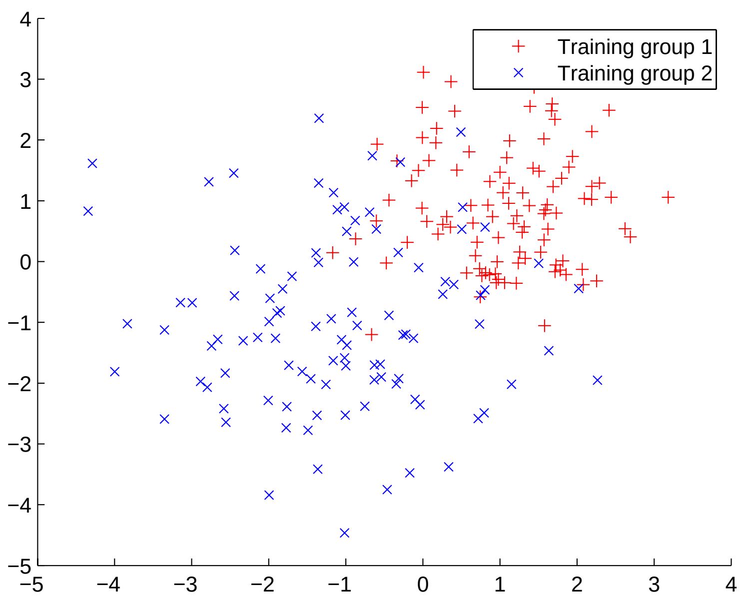
```
sample = [.9 .8;.1 .3;.2 .6]

sample =
    0.9000    0.8000
    0.1000    0.3000
    0.2000    0.6000

training=[0 0;.5 .5;1 1]

training =
         0         0
    0.5000    0.5000
    1.0000    1.0000

group = [1;2;3]

group =
     1
     2
     3

class = knnclassify(sample, training, group)

class =
     3
     1
     2
```

Row 1 of `sample` is closest to row 3 of `Training`, so `class(1) = 3`. Row 2 of `sample` is closest to row 1 of `Training`, so `class(2) = 1`. Row 3 of `sample` is closest to row 2 of `Training`, so `class(3) = 2`.

Classifying Rows into One of Two Groups

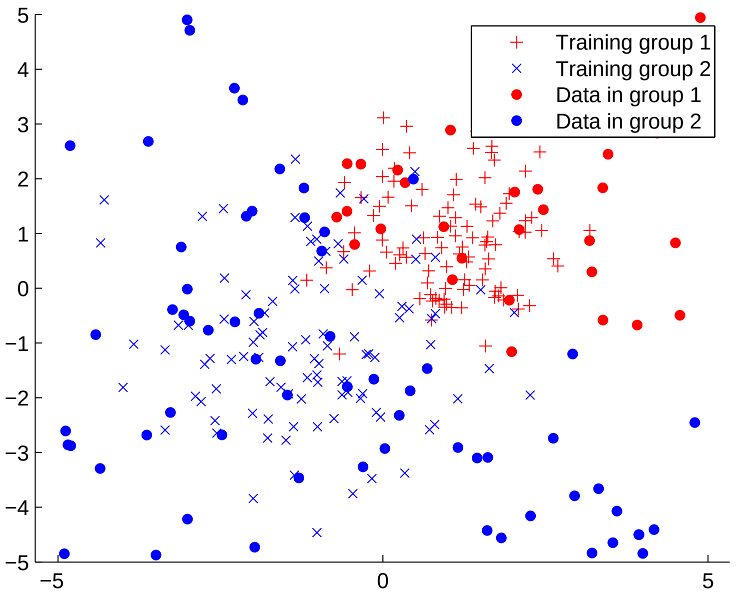
The following example classifies each row of the data in `sample` into one of the two groups in `training`. The following commands create the matrix `training` and the grouping variable `group`, and plot the rows of `training` in two groups.

```
training = [mvnrnd([ 1  1],   eye(2), 100); ...
            mvnrnd([-1 -1], 2*eye(2), 100)];
group = [repmat(1,100,1); repmat(2,100,1)];
gscatter(training(:,1),training(:,2),group,'rb','+x');
legend('Training group 1', 'Training group 2');
hold on;
```



The following commands create the matrix `sample`, classify its rows into two groups, and plot the result.

```
sample = unifrnd(-5, 5, 100, 2);
% Classify the sample using the nearest neighbor classification
c = knnclassify(sample, training, group);
gscatter(sample(:,1),sample(:,2),c,'mc'); hold on;
legend('Training group 1','Training group 2', ...
       'Data in group 1','Data in group 2');
hold off;
```

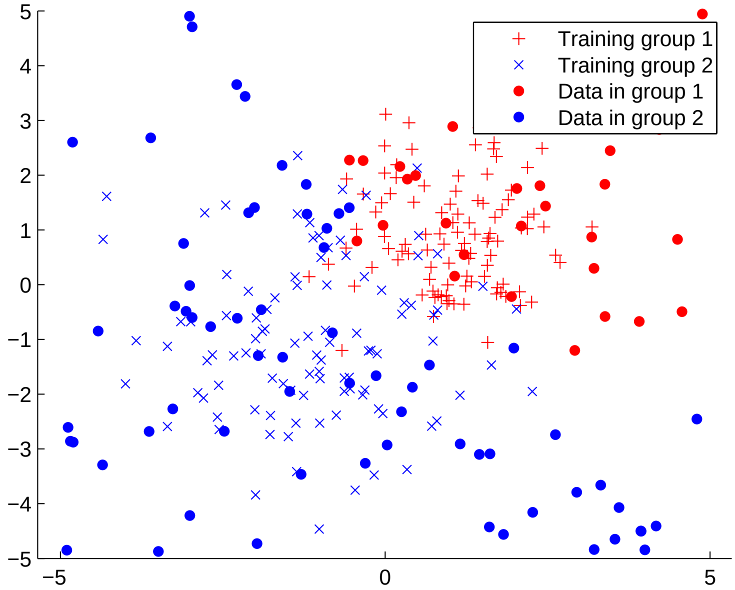


Classifying Rows Using the Three Nearest Neighbors

The following example uses the same data as in Example 2, but classifies the rows of `sample` using three nearest neighbors instead of one.

```
gscatter(training(:,1),training(:,2),group,'rb',+x');
hold on;
c3 = knnclassify(sample, training, group, 3);
```

```
gscatter(sample(:,1),sample(:,2),c3,'mc','o');
legend('Training group 1','Training group 2','Data in group 1','Data in group 2');
```



If you compare this plot with the one in Example 2, you see that some of the data points are classified differently using three nearest neighbors.

References

[1] Mitchell T (1997), Machine Learning, McGraw-Hill.

See Also

Bioinformatics Toolbox functions: `knnimpute`, `classperf`, `crossvalind`, `svmclassify`, `svmtrain`

Statistics Toolbox functions: `classify`

knnimpute

Purpose

Impute missing data using nearest-neighbor method

Syntax

```
knnimpute(Data)
knnimpute(Data, k)
knnimpute(..., 'PropertyName', PropertyValue,...)
knnimpute(..., 'Distance', DistanceValue)
knnimpute(..., 'DistArgs', DistArgsValue)
knnimpute(..., 'Weights', WeightsValues)
knnimpute(..., 'Median', MedianValue)
```

Arguments

Data

k

Description

`knnimpute(`*`Data`*`)`replaces `NaN`s in `Data` with the corresponding value from the nearest-neighbor column. The nearest-neighbor column is the closest column in Euclidean distance. If the corresponding value from the nearest-neighbor column is also `NaN`, the next nearest column is used.

`knnimpute(`*`Data`*`, `*`k`*`)`replaces `NaN`s in `Data` with a weighted mean of the `k` nearest-neighbor columns. The weights are inversely proportional to the distances from the neighboring columns.

`knnimpute(..., '`*`PropertyName`*`', `*`PropertyValue`*`,...)` defines optional properties using property name/value pairs.

`knnimpute(..., 'Distance', `*`DistanceValue`*`)` computes nearest-neighbor columns using the distance metric `distfun`. The choices for *`DistanceValue`* are

`'euclidean'`	Euclidean distance (default).
`'seuclidean'`	Standardized Euclidean distance — each coordinate in the sum of squares is inversely weighted by the sample variance of that coordinate.

`'cityblock'`	City block distance
`'mahalanobis'`	Mahalanobis distance
`'minkowski'`	Minkowski distance with exponent 2
`'cosine'`	One minus the cosine of the included angle
`'correlation'`	One minus the sample correlation between observations, treated as sequences of values
`'hamming'`	Hamming distance — the percentage of coordinates that differ
`'jaccard'`	One minus the Jaccard coefficient — the percentage of nonzero coordinates that differ
`'chebychev'`	Chebychev distance (maximum coordinate difference)
function handle	A handle to a distance function, specified using `@`, for example `@distfun`

See `pdist` for more details.

`knnimpute(..., 'DistArgs', `*`DistArgsValue`*`)` passes arguments (*`DistArgsValue`*) to the function `distfun`. *`DistArgsValue`* can be a single value or a cell array of values.

`knnimpute(..., 'Weights', `*`WeightsValues`*`)` enables you to specify the weights used in the weighted mean calculation. `w` should be a vector of length `k`.

`knnimpute(..., 'Median', `*`MedianValue`*`)` when MedianValue is `true`, uses the median of the `k` nearest neighbors instead of the weighted mean.

Example 1

```
A = [1 2 5;4 5 7;NaN -1 8;7 6 0]

A =

     1     2     5
     4     5     7
```

```
NaN    -1     8
  7     6     0
```

Note that `A(3,1) = NaN`. Because column 2 is the closest column to column 1 in Euclidean distance, `knnimpute` imputes the `(3,1)` entry of column 1 to be the corresponding entry of column 2, which is `-1`.

```
knnimpute(A)

ans =

     1     2     5
     4     5     7
    -1    -1     8
     7     6     0
```

Example 2

The following example loads the data set `yeastdata` and imputes missing values in the array `yeastvalues`.

```
load yeastdata
% Remove data for empty spots
emptySpots = strcmp('EMPTY',genes);
yeastvalues(emptySpots,:) = [];
genes(emptySpots) = [];
% Impute missing values
imputedValues = knnimpute(yeastvalues);
```

References

[1] Speed T (2003), *Statistical Analysis of Gene Expression Microarray Data*, Chapman & Hall/CRC.

[2] Hastie T, Tibshirani R, Sherlock G. Eisen M, Brown P, Botstein D (1999), “Imputing missing data for gene expression arrays”, Technical Report, Division of Biostatistics, Stanford University.

[3] Troyanskaya O, Cantor M, Sherlock G, Brown P, Hastie T, Tibshirani R, Botstein D, Altman R (2001), “Missing value estimation methods for DNA microarrays”, Bioinformatics, 17(6)520-525.

See Also

Bioinformatics Toolbox function `knnclassify`

MATLAB function `isnan`

Statistics Toolbox functions `nanmean`, `nanmedian`, `pdist`

maboxplot

Purpose Box plot for microarray data

Syntax

```
maboxplot(MAData)
maboxplot(MAData, ColumnName)
maboxplot(MAStruct, FieldName)
H = maboxplot(...)
[H, HLines] = maboxplot(...)
maboxplot(..., 'PropertyName', PropertyValue, ...)
maboxplot(..., 'Title', TitleValue, ...)
maboxplot(..., 'Notch', NotchValue, ...)
maboxplot(..., 'Symbol', SymbolValue, ...)
maboxplot(..., 'Orientation', OrientationValue, ...)
maboxplot(..., 'WhiskerLength', WhiskerLengthValue, ...)
```

Arguments

MAData	A numeric array or a structure containing a field called `Data`. The values in the columns of *MAData* will be used to create box plots.
ColumnName	An array of column names corresponding to the data in *MAData*.
MAStruct	A microarray data structure.
FieldName	A field within the microarray data structure, *MAStruct*. The values in the field *FieldName* will be used to create box plots.
TitleValue	A string to use as the title for the plot. The default title is `FieldName`.
NotchValue	Property to control the type of boxes drawn. Enter either `true` for notched boxes, or `false`, for square boxes. Default is `false`.

OrientationValue	Property to specify the orientation of the box plot. Enter `'Vertical'` or `'Horizontal'`. Default is `'Horizontal'`.
WhiskerLengthValue	Property to specify the maximum length of the whiskers as a function of the interquartile range (IQR). The whisker extends to the most extreme data value within *WhiskerLengthValue*`*IQR` of the box. Default = `1.5`. If *WhiskerLengthValue* equals `0`, then `maboxplot` displays all data values outside the box, using the plotting symbol `Symbol`.

Description

`maboxplot(`*MAData*`)` displays a box plot of the values in the columns of data (*MAData*). *MAData* can be a numeric array or a structure containing a field called `Data`.

`maboxplot(`*MAData, ColumnName*`)` labels the box plot column names.

`maboxplot(`*MAStruct, FieldName*`)` displays a box plot of the values in the field `FieldName` in the microarray data structure *MAStruct*. If *MAStruct* is block based, `maboxplot` creates a box plot of the values in the field *FieldName* for each block.

H `= maboxplot(...)` returns the handle of the box plot axes.

`[`*H*`, `*HLines*`] = maboxplot(...)` returns the handles of the lines used to separate the different blocks in the image.

`maboxplot(..., '`*PropertyName*`', `*PropertyValue*`, ...)` defines optional properties using property name/value pairs in any order. These property name/value pairs are as follows:

`maboxplot(..., 'Title', `*TitleValue*`, ...)` allows you to specify the title of the plot. The default *TitleValue* is `FieldName`.

`maboxplot(..., 'Notch', `*NotchValue*`, ...)` if *NotchValue* is `true`, draws notched boxes. The default is `false` to show square boxes.

`maboxplot(..., 'Symbol', SymbolValue, ...)` allows you to specify the symbol used for outlier values. The default `Symbol` is `'+'`.

`maboxplot(..., 'Orientation', OrientationValue, ...)` allows you to specify the orientation of the box plot. The choices are `'Vertical'` and `'Horizontal'`. The default is `'Vertical'`.

`maboxplot(..., 'WhiskerLength', WhiskerLengthValue, ...)` allows you to specify the whisker length for the box plot. *`WhiskerLengthValue`* defines the maximum length of the whiskers as a function of the interquartile range (IQR) (default = `1.5`). The whisker extends to the most extreme data value within `WhiskerLength*IQR` of the box. If *`WhiskerLengthValue`* equals `0`, then `maboxplot` displays all data values outside the box, using the plotting symbol `Symbol`.

Examples

```
load yeastdata
maboxplot(yeastvalues,times);
xlabel('Sample Times');

% Using a structure
geoStruct = getgeodata('GSM1768');
maboxplot(geoStruct);

% For block-based data
madata = gprread('mouse_a1wt.gpr');
maboxplot(madata,'F635 Median');
figure
maboxplot(madata,'F635 Median - B635','TITLE',...
          'Cy5 Channel FG - BG');
```

See Also

Bioinformatics Toolbox functions `magetfield`, `maimage`, `mairplot`, `maloglog`, `malowess`, `manorm`, `mavolcanoplot`

Statistics Toolbox function `boxplot`

Purpose

Estimate false discovery rate (FDR) of differentially expressed genes from two experimental conditions or phenotypes

Syntax

```
FDR = mafdr(PValues)
[FDR, Q] = mafdr(PValues)
[FDR, Q, Pi0] = mafdr(PValues)
[FDR, Q, Pi0, R2] = mafdr(PValues)
... = mafdr(PValues, ...'BHFDR', BHFDRValue, ...)
... = mafdr(PValues, ...'Lambda', LambdaValue, ...)
... = mafdr(PValues, ...'Method', MethodValue, ...)
... = mafdr(PValues, ...'Showplot', ShowplotValue, ...)
```

Arguments

PValues	Column vector of p-values for each gene in two microarray data sets, such as returned by `mattest`.
BHFDRValue	Property to control the use of the linear step-up (LSU) procedure originally introduced by Benjamini and Hochberg, 1995. Choices are `true` or `false` (default).

Note If *BHFDRValue* is set to `true`, the `Lambda` and `Method` properties are ignored.

`LambdaValue` Input that specifies lambda, λ, the tuning parameter used to estimate the true null hypotheses, $\hat{\pi}_0(\lambda)$. *`LambdaValue`* can be either:

- A single value that is `> 0` and `< 1`.
- A series of values. Each value must be `> 0` and `< 1`. There must be at least four values in the series.

> **Tip** The series of values can be expressed by a colon operator with the form `[`*`first`*`:`*`incr`*`:`*`last`*`]`, where *`first`* is the first value in the series, *`incr`* is the increment, and *`last`* is the last value in the series.

Default *`LambdaValue`* is the series of values `[0.01:0.01:0.95]`.

> **Note** If *`LambdaValue`* is set to a single value, the `Method` property is ignored.

MethodValue	String that specifies a method to calculate the true null hypothesis, $\hat{\pi}_0(\lambda)$, from the tuning parameter, *LambdaValue*, when *LambdaValue* is a series of values. Choices are: • `bootstrap` (default) • `polynomial`
ShowplotValue	Property to display two plots: • Plot of the estimated true null hypotheses, $\hat{\pi}_0(\lambda)$, versus the tuning parameter, lambda, λ, with a cubic polynomial fitting curve • Plot of q-values versus p-values Choices are `true` or `false` (default).

Return Values

FDR	Column vector of positive FDR (pFDR) values.
Q	Column vector of q-values.
Pi0	Estimated true null hypothesis, $\hat{\pi}_0$.
R2	Square of the correlation coefficient.

Description

`FDR = mafdr(PValues)` computes a positive FDR (pFDR) value for each value in *PValues*, a column vector of p-values for each gene in two microarray data sets, using a procedure introduced by Storey, 2002. *FDR* is a column vector of positive FDR (pFDR) values.

`[FDR, Q] = mafdr(PValues)` also returns a q-value for each p-value in *PValues*. *Q* is a column vector.

[*FDR*, *Q*, *Pi0*] = mafdr(*PValues*) also returns *Pi0*, the estimated true null hypothesis, $\hat{\pi}_0$, if using the procedure introduced by Storey, 2002.

[*FDR*, *Q*, *Pi0*, *R2*] = mafdr(*PValues*) also returns *R2*, the square of the correlation coefficient, if using the procedure introduced by Storey, 2002, and the polynomial method to calculate the true null hypothesis, $\hat{\pi}_0$, from the tuning parameter, lambda, λ.

... = mafdr(*PValues*, ...'*PropertyName*', *PropertyValue*, ...) calls mafdr with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

... = mafdr(*PValues*, ...'BHFDR', *BHFDRValue*, ...) controls the use of the linear step-up (LSU) procedure originally introduced by Benjamini and Hochberg, 1995, to computes an FDR-adjusted p-value for each value in *PValues*. Choices are true or false (default).

Note If *BHFDRValue* is set to true, the Lambda and Method properties are ignored.

... = mafdr(*PValues*, ...'Lambda', *LambdaValue*, ...) specifies lambda, λ, the tuning parameter used to estimate the true null hypotheses, $\hat{\pi}_0(\lambda)$. *LambdaValue* can be either:

- A single value that is > 0 and < 1.
- A series of values. Each value must be > 0 and < 1. There must be at least four values in the series.

Tip The series of values can be expressed by a colon operator with the form `[`*`first`*`:`*`incr`*`:`*`last`*`]`, where *`first`* is the first value in the series, *`incr`* is the increment, and *`last`* is the last value in the series.

Default *`LambdaValue`* is the series of values `[0.01:0.01:0.95]`.

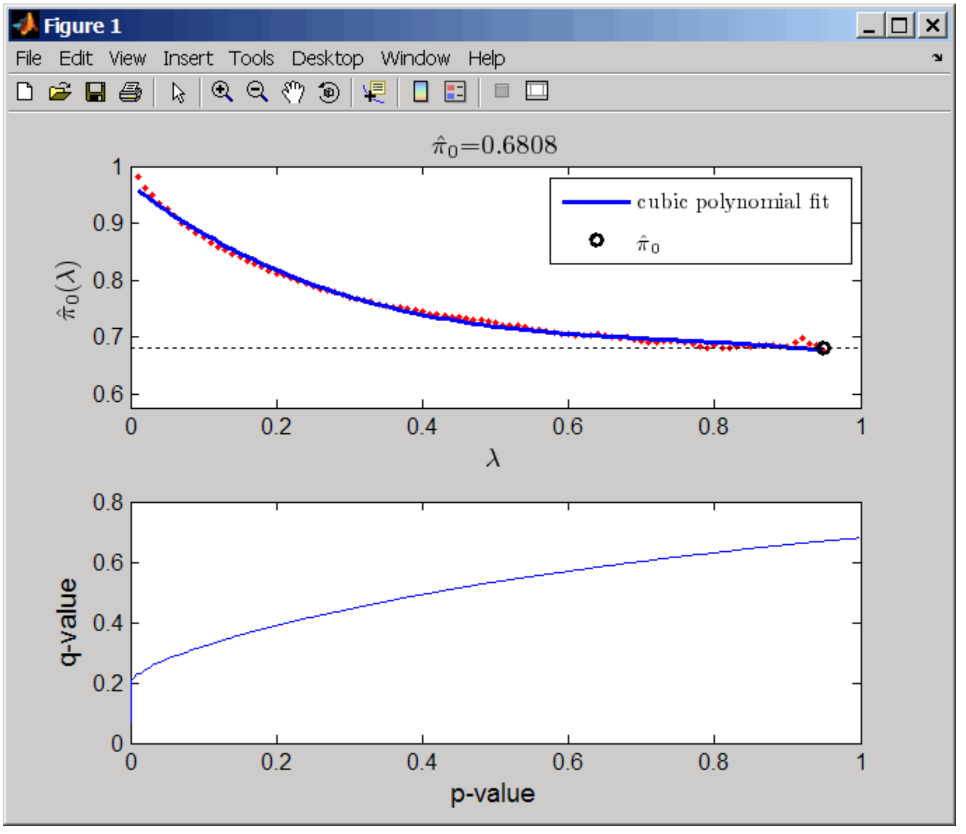
Note If *`LambdaValue`* is set to a single value, the `Method` property is ignored.

`... = mafdr(`*`PValues`*`, ...'Method', `*`MethodValue`*`, ...)` specifies a method to calculate the true null hypothesis, $\hat{\pi}_0$, from the tuning parameter, *`LambdaValue`*, when *`LambdaValue`* is a series of values. Choices are `bootstrap` (default) or `polynomial`.

`... = mafdr(`*`PValues`*`, ...'Showplot', `*`ShowplotValue`*`, ...)` controls the display of two plots:

- Plot of the estimated true null hypotheses, $\hat{\pi}_0(\lambda)$, versus the tuning parameter, lambda, with a cubic polynomial fitting curve
- Plot of q-values versus p-values

Choices are `true` or `false` (default).



Examples

1 Load the MAT file, included with Bioinformatics Toolbox, that contains Affymetrix data from a prostate cancer study, specifically probe intensity data from Affymetrix HG-U133A GeneChip arrays. The two variables in the MAT file, `dependentData` and `independentData`, are two matrices of gene expression values from two experimental conditions.

```
load prostatecancerexpdata
```

2 Use the `mattest` function to calculate p-values for the gene expression values in the two matrices.

```
pvalues = mattest(dependentData, independentData, 'permute', true);
```

3 Use the `mafdr` function to calculate positive FDR values and q-values for the gene expression values in the two matrices and plot the data.

```
[fdr, q] = mafdr(pvalues, 'showplot', true);
```

The `prostatecancerexpdata.mat` file used in this example contains data from Best et al., 2005.

References

[1] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

[2] Storey, J.D. (2002). A direct approach to false discovery rates. Journal of the Royal Statistical Society *64(3)*, 479–498.

[3] Storey, J.D., and Tibshirani, R. (2003). Statistical significance for genomewide studies. Proc Nat Acad Sci *100(16)*, 9440–9445.

[4] Storey, J.D., Taylor, J.E., and Siegmund, D. (2004). Strong control conservative point estimation and simultaneous conservative consistency of false discovery rates: A unified approach. Journal of the Royal Statistical Society *66*, 187–205.

[5] Benjamini, Y., and Hochberg, Y. (1995). Controlling the false discovery rate: A practical and powerful approach to multiple testing. Journal of the Royal Statistical Society *57*, 289–300.

See Also

Bioinformatics Toolbox functions: `gcrma`, `mairplot`, `maloglog`, `mapcaplot`, `mattest`, `mavolcanoplot`, `rmasummary`

magetfield

Purpose Extract data from microarray structure

Syntax `magetfield(MAStruct, FieldName)`

Arguments

`MAStruct`

`FieldName`

Description `magetfield(MAStruct, FieldName)` extracts data for a column (*`FieldName`*) from a microarray structure (*`MAStruct`*).

The benefit of this function is to hide the details of extracting a column of data from a structure created with one of the microarray reader functions (`gprread`, `agferead`, `sptread`, `imageneread`).

Examples

```
maStruct = gprread('mouse_a1wt.gpr');
cy3data = magetfield(maStruct,'F635 Median');
cy5data = magetfield(maStruct,'F532 Median');
mairplot(cy3data,cy5data,'title','R vs G IR plot');
```

See Also Bioinformatics Toolbox functions `agferead`, `gprread`, `imageneread`, `maboxplot`, `mairplot`, `maloglog`, `malowess`, `sptread`

Purpose

Spatial image for microarray data

Syntax

```
maimage(X, FieldName)
H = maimage(...)
[H, HLines] = maimage(...)
maimage(..., 'PropertyName', PropertyValue,...)
maimage(..., 'Title', TitleValue)
maimage(..., 'ColorBar', ColorBarValue)
maimage(..., 'HandleGraphicsPropertyName' PropertyValue)
```

Arguments

X	A microarray data structure.
FieldName	A field in the microarray data structure *X*.
TitleValue	A string to use as the title for the plot. The default title is `FieldName`.
ColorBarValue	Property to control displaying a color bar in the figure window. Enter either `true` or `false`. The default value is `false`.

Description

`maimage(X, FieldName)` displays an image of field *FieldName* from microarray data structure *X*. Microarray data can be GenPix Results (GPR) format. After creating the image, click a data point to display the value and ID, if known.

`H = maimage(...)` returns the handle of the image.

`[H, HLines] = maimage(...)` returns the handles of the lines used to separate the different blocks in the image.

`maimage(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`maimage(..., 'Title', TitleValue)` allows you to specify the title of the plot. The default title is `FieldName`.

`maimage(..., 'ColorBar', ColorBarValue)`, when *ColorBarValue* is `true`, a color bar is shown. If *ColorBarValue* is `false`, no color bar is shown. The default is for the color bar to be shown.

`maimage(..., 'HandleGraphicsPropertyName' PropertyValue)` allows you to pass optional Handle Graphics® property name/value pairs to the function. For example, a name/value pair for color could be `maimage(..., 'color' 'r')`.

Examples

```
madata = gprread('mouse_a1wt.gpr');
maimage(madata,'F635 Median');
figure;
maimage(madata,'F635 Median - B635',...
        'Title','Cy5 Channel FG - BG');
colormap hot
```

See Also

Bioinformatics Toolbox functions: `maboxplot`, `magetfield`, `mairplot`, `maloglog`, `malowess`

MATLAB function: `imagesc`

Purpose

Perform rank invariant set normalization on gene expression values from two experimental conditions or phenotypes

Syntax

```
NormDataY = mainvarsetnorm(DataX, DataY)
NormDataY = mainvarsetnorm(..., 'Thresholds',
ThresholdsValue, ...)
NormDataY = mainvarsetnorm(..., 'Exclude',
ExcludeValue, ...)
NormDataY = mainvarsetnorm(..., 'Prctile',
PrctileValue, ...)
NormDataY = mainvarsetnorm(..., 'Iterate',
IterateValue, ...)
NormDataY = mainvarsetnorm(..., 'Method', MethodValue, ...)
NormDataY = mainvarsetnorm(..., 'Span', SpanValue, ...)
NormDataY = mainvarsetnorm(..., 'Showplot', ShowplotValue,
    ...)
```

Arguments

DataX	Vector of gene expression values from a single experimental condition or phenotype, where each row corresponds to a gene. These data points are used as the baseline.
DataY	Vector of gene expression values from a single experimental condition or phenotype, where each row corresponds to a gene. These data points will be normalized using the baseline.

ThresholdsValue	Property to set the thresholds for the lowest average rank and the highest average rank, which are used to determine the invariant set. The rank invariant set is a set of data points whose proportional rank difference is smaller than a given threshold. The threshold for each data point is determined by interpolating between the threshold for the lowest average rank and the threshold for the highest average rank. Select these two thresholds empirically to limit the spread of the invariant set, but allow enough data points to determine the normalization relationship. *ThresholdsValue* is a 1-by-2 vector [*LT, HT*], where *LT* is the threshold for the lowest average rank and *HT* is threshold for the highest average rank. Values must be between `0` and `1`. Default is [`0.03, 0.07`].
ExcludeValue	Property to filter the invariant set of data points, by excluding the data points whose average rank (between *DataX* and *DataY*) is in the highest *N* ranked averages or lowest *N* ranked averages.
PrctileValue	Property to stop the iteration process when the number of data points in the invariant set reaches *N* percent of the total number of input data points. Default is `1`. **Note** If you do not use this property, the iteration process continues until no more data points are eliminated.

IterateValue	Property to control the iteration process for determining the invariant set of data points. Enter `true` to repeat the process until either no more data points are eliminated, or a predetermined percentage of data points (*StopPrctileValue*) is reached. Enter `false` to perform only one iteration of the process. Default is `true`. **Tip** Select `false` for smaller data sets, typically less than 200 data points.
MethodValue	Property to select the smoothing method used to normalize the data. Enter `'lowess'` or `'runmedian'`. Default is `'lowess'`.
SpanValue	Property to set the window size for the smoothing method. If *SpanValue* is less than 1, the window size is that percentage of the number of data points. If *SpanValue* is equal to or greater than 1, the window size is of size *SpanValue*. Default is `0.05`, which corresponds to a window size equal to 5% of the total number of data points in the invariant set.
ShowplotValue	Property to control the plotting of a pair of M-A scatter plots (before and after normalization). M is the ratio between *DataX* and *DataY*. A is the average of *DataX* and *DataY*. Enter `true` to create the pair of M-A scatter plots. Default is `false`.

Description

`NormDataY = mainvarsetnorm(DataX, DataY)` normalizes the values in *DataY*, a vector of gene expression values, to a reference vector, *DataX*, using the invariant set method. *NormDataY* is a vector of normalized gene expression values from *DataY*.

Specifically, `mainvarsetnorm`:

- Determines the proportional rank difference (*prd*) for each pair of ranks, *RankX* and *RankY*, from the two vectors of gene expression values, *`DataX`* and *`DataY`*.

  prd = abs(*RankX* - *RankY*)

- Determines the invariant set of data points by selecting data points whose proportional rank differences (*prd*) are below *threshold*, which is a predetermined threshold for a given data point (defined by the *`ThresholdsValue`* property). It optionally repeats the process until either no more data points are eliminated, or a predetermined percentage of data points is reached.

  The invariant set is data points with a *prd* < *threshold*.

- Uses the invariant set of data points to calculate the lowess or running median smoothing curve, which is used to normalize the data in *`DataY`*.

Note If *`DataX`* or *`DataY`* contains NaN values, then *`NormDataY`* will also contain NaN values at the corresponding positions.

Tip `mainvarsetnorm` is useful for correcting for dye bias in two-color microarray data.

`NormDataY` `= mainvarsetnorm(..., '`*`PropertyName`*`',` *`PropertyValue`*`, ...)` defines optional properties that use property name/value pairs in any order. These property name/value pairs are as follows:

`NormDataY = mainvarsetnorm(..., 'Thresholds', ThresholdsValue, ...)` sets the thresholds for the lowest average rank and the highest average rank, which are used to determine the invariant set. The rank invariant set is a set of data points whose proportional rank difference is smaller than a given threshold. The threshold for each data point is determined by interpolating between the threshold for the lowest average rank and the threshold for the highest average rank. Select these two thresholds empirically to limit the spread of the invariant set, but allow enough data points to determine the normalization relationship.

ThresholdsValue is a 1-by-2 vector [*LT, HT*], where *LT* is the threshold for the lowest average rank and *HT* is threshold for the highest average rank. Values must be between `0` and `1`. Default is [`0.03, 0.07`].

`NormDataY = mainvarsetnorm(..., 'Exclude', ExcludeValue, ...)` filters the invariant set of data points, by excluding the data points whose average rank (between *DataX* and *DataY*) is in the highest *N* ranked averages or lowest *N* ranked averages.

`NormDataY = mainvarsetnorm(..., 'Prctile', PrctileValue, ...)` stops the iteration process when the number of data points in the invariant set reaches *N* percent of the total number of input data points. Default is `1`.

Note If you do not use this property, the iteration process continues until no more data points are eliminated.

`NormDataY = mainvarsetnorm(..., 'Iterate', IterateValue, ...)` controls the iteration process for determining the invariant set of data points. When *IterateValue* is `true`, `mainvarsetnorm` repeats the process until either no more data points are eliminated, or a predetermined percentage of data points (*PrctileValue*) is reached. When *IterateValue* is `false`, performs only one iteration of the process. Default is `true`.

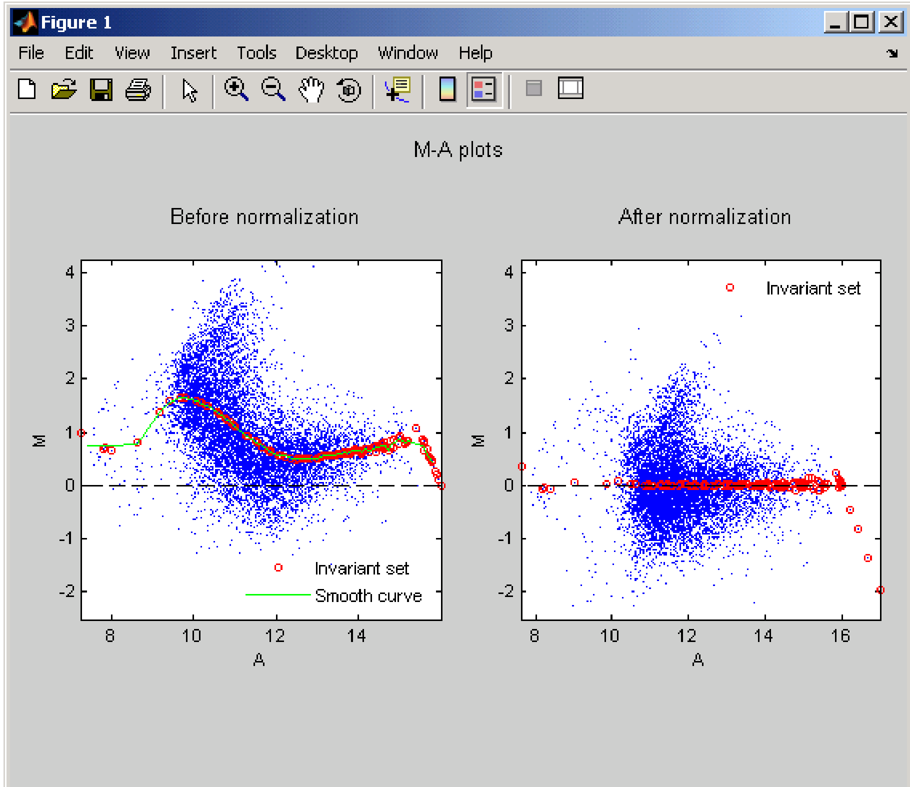
Tip Select `false` for smaller data sets, typically less than 200 data points.

`NormDataY = mainvarsetnorm(..., 'Method', MethodValue, ...)` selects the smoothing method for normalizing the data. When `MethodValue` is `'lowess'`, `mainvarsetnorm` uses the lowess method. When `MethodValue` is `'runmedian'`, `mainvarsetnorm` uses the running median method. Default is `'lowess'`.

`NormDataY = mainvarsetnorm(..., 'Span', SpanValue, ...)` sets the window size for the smoothing method. If `SpanValue` is less than 1, the window size is that percentage of the number of data points. If `SpanValue` is equal to or greater than 1, the window size is of size `SpanValue`. Default is `0.05`, which corresponds to a window size equal to 5% of the total number of data points in the invariant set.

`NormDataY = mainvarsetnorm(..., 'Showplot', ShowplotValue, ...)` determines whether to plot a pair of M-A scatter plots (before and after normalization). M is the ratio between `DataX` and `DataY`. A is the average of `DataX` and `DataY`. When `ShowplotValue` is `true`, `mainvarsetnorm` plots the M-A scatter plots. Default is `false`.

The following example illustrates how `mainvarsetnorm` can correct for dye bias or scanning differences between two channels of data from a two-color microarray experiment. Under perfect experimental conditions, data points with equal expression values would fall along the M = 0 line, which represents a gene expression ratio of 1. However, dye bias caused the measured values in one channel to be higher than the other channel, as seen in the Before Normalization plot. Normalization corrected the variance, as seen in the After Normalization plot.



Examples

The following example extracts data from a GPR file and creates two column vectors of gene expression values from different experimental conditions. It then normalizes one of the data sets.

```
maStruct = gprread('mouse_a1wt.gpr');
cy3data = magetfield(maStruct, 'F635 Median');
cy5data = magetfield(maStruct, 'F532 Median');
Normcy5data = mainvarsetnorm(cy3data, cy5data);
```

References

[1] Tseng, G.C., Oh, Min-Kyu, Rohlin, L., Liao, J.C., and Wong, W.H. (2001) Issues in cDNA microarray analysis: quality filtering, channel

normalization, models of variations and assessment of gene effects. Nucleic Acids Research. *29*, 2549-2557.

[2] Hoffmann, R., Seidl, T., and Dugas, M. (2002) Profound effect of normalization on detection of differentially expressed genes in oligonucleotide microarray data analysis. Genome Biology. *3(7)*: research 0033.1-0033.11.

See Also

`affyinvarsetnorm`, `malowess`, `manorm`, `quantilenorm`

Purpose

Create intensity versus ratio scatter plot of microarray data

Syntax

```
mairplot(DataX, DataY)
[Intensity, Ratio] = mairplot(DataX, DataY)
[Intensity, Ratio, H] = mairplot(DataX, DataY)
mairplot(..., 'Type', TypeValue, ...)
mairplot(..., 'LogTrans', LogTransValue, ...)
mairplot(..., 'FactorLines', FactorLinesValue, ...)
mairplot(..., 'Title', TitleValue, ...)
mairplot(..., 'Labels', LabelsValue, ...)
mairplot(..., 'Normalize', NormalizeValue, ...)
mairplot(..., 'LowessOptions', LowessOptionsValue, ...)
```

Arguments

DataX, *DataY*	Vectors of gene expression values where each row corresponds to a gene. For example, in a two-color microarray experiment, *DataX* could be cy3 intensity values and *DataY* could be cy5 intensity values.
TypeValue	String that specifies the plot type. Choices are `'IR'` (plots $\log_{10}$ of the product of the *DataX* and *DataY* intensities versus $\log_2$ of the intensity ratios) or `'MA'` (plots (1/2)$\log_2$ of the product of the *DataX* and *DataY* intensities versus $\log_2$ of the intensity ratios). Default is `'IR'`.
LogTransValue	Controls the conversion of data in *X* and *Y* from natural scale to $\log_2$ scale. Set *LogTransValue* to `false`, when the data is already $\log_2$ scale. Default is `true`, which assumes the data is natural scale.

FactorLinesValue	Adds lines to the plot showing a factor of *N* change. Default is 2, which corresponds to a level of 1 and -1 on a $\log_2$ scale.

> **Tip** You can also change the factor lines interactively, after creating the plot.

TitleValue	String that specifies a title for the plot.
LabelsValue	Cell array of labels for the data. If labels are defined, then clicking a point on the plot shows the label corresponding to that point.
NormalizeValue	Controls the display of lowess normalized ratio values. Enter `true` to display to lowess normalized ratio values. Default is `false`.

> **Tip** You can also normalize the data from the MAIR Plot window, after creating the plot.

LowessOptionsValue — Cell array of one, two, or three property name/value pairs in any order that affect the lowess normalization. Choices for property name/value pairs are:

- `'Order'`, *OrderValue*
- `'Robust'`, *RobustValue*
- `'Span'`, *SpanValue*

For more information on the preceding property name/value pairs, see `malowess`.

Return Values

Intensity	Vector containing intensity values for the microarray gene expression data, calculated as: • $\log_{10}$ of the product of the *DataX* and *DataY* intensities (when `Type` is `'IR'`) • $(1/2)\log_2$ of the product of the *DataX* and *DataY* intensities (when `Type` is `'MA'`)
Ratio	Vector containing ratios of the microarray gene expression data, calculated as `log2(`*DataX*`./`*DataY*`)`.
H	Handle of the plot.

Description

`mairplot(`*DataX*`, `*DataY*`)` creates a scatter plot that plots $\log_{10}$ of the product of the *DataX* and *DataY* intensities versus $\log_2$ of the intensity ratios.

`[`*Intensity*`, `*Ratio*`] = mairplot(`*DataX*`, `*DataY*`)` returns the intensity and ratio values. If you set `'Normalize'` to `true`, the returned ratio values are normalized.

`[`*Intensity*`, `*Ratio*`, `*H*`] = mairplot(`*DataX*`, `*DataY*`)` returns the handle of the plot.

`...  = mairplot(..., '`*PropertyName*`', `*PropertyValue*`, ...)` calls `mairplot` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`mairplot(..., 'Type', `*TypeValue*`, ...)` specifies the plot type. Choices are `'IR'` (plots $\log_{10}$ of the product of the *DataX* and *DataY* intensities versus $\log_2$ of the intensity ratios) or `'MA'` (plots $(1/2)\log_2$ of the product of the *DataX* and *DataY* intensities versus $\log_2$ of the intensity ratios). Default is `'IR'`.

`mairplot(..., 'LogTrans', LogTransValue, ...)` controls the conversion of data in *X* and *Y* from natural to $\log_2$ scale. Set *`LogTransValue`* to `false`, when the data is already $\log_2$ scale. Default is `true`, which assumes the data is natural scale.

`mairplot(..., 'FactorLines', FactorLinesValue, ...)` adds lines to the plot showing a factor of *N* change. Default is 2, which corresponds to a level of 1 and -1 on a $\log_2$ scale.

Tip You can also change the factor lines interactively, after creating the plot.

`mairplot(..., 'Title', TitleValue, ...)` specifies a title for the plot.

`mairplot(..., 'Labels', LabelsValue, ...)` specifies a cell array of labels for the data. If labels are defined, then clicking a point on the plot shows the label corresponding to that point.

`mairplot(..., 'Normalize', NormalizeValue, ...)` controls the display of lowess normalized ratio values. Enter `true` to display to lowess normalized ratio values. Default is `false`.

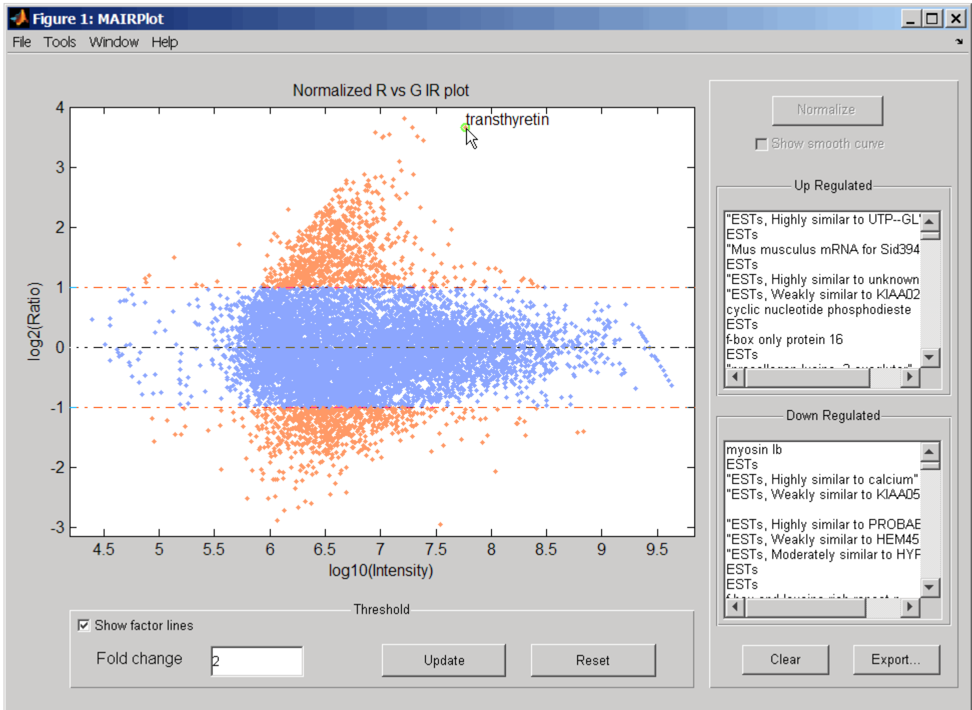
Tip You can also normalize the data from the MAIR Plot window, after creating the plot.

`mairplot(..., 'LowessOptions', LowessOptionsValue, ...)` lets you specify up to three property name/value pairs (in any order) that affect the lowess normalization. Choices for property name/value pairs are:

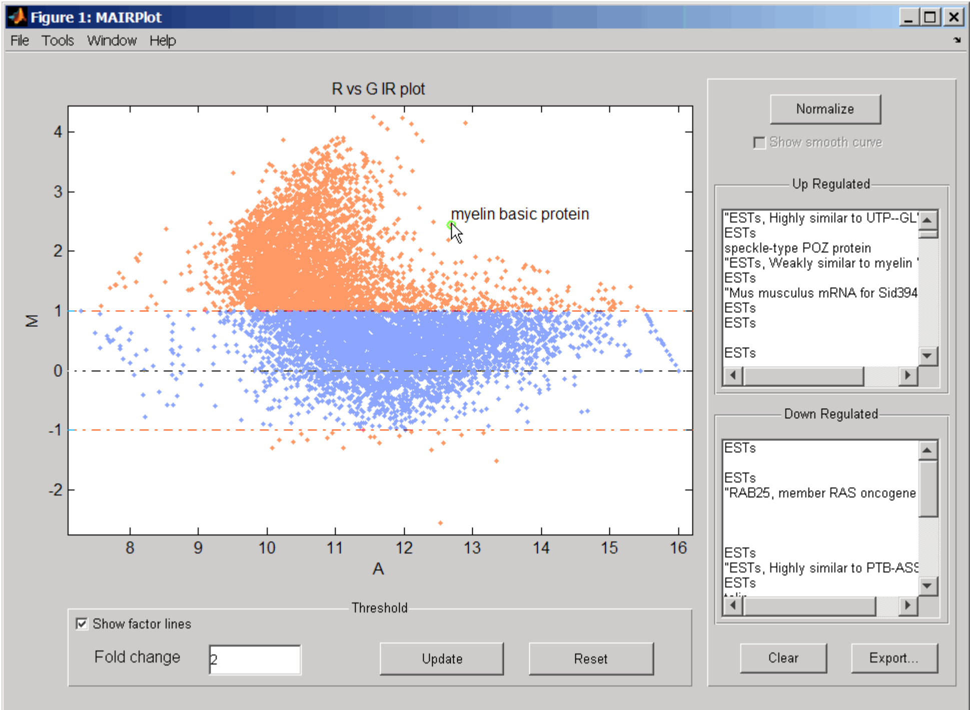
- `'Order', OrderValue`
- `'Robust', RobustValue`
- `'Span', SpanValue`

For more information on the previous three property name/value pairs, see the `malowess` function.

Following is an IR plot of normalized data.



Following is an M-A plot of unnormalized data.



The intensity versus ratio scatter plot displays the following:

- $\log_{10}$ (Intensity) versus $\log_2$ (Ratio) scatter plot of genes.
- Two horizontal fold change lines at a fold change level of 2, which corresponds to a ratio of 1 and –1 on a $\log_2$ (Ratio) scale. (Lines will be at different fold change levels, if you used the `'FactorLines'` property.)
- Data points for genes that are considered differentially expressed (outside of the fold change lines) appear in orange.

After you display the intensity versus ratio scatter plot, you can interactively do the following:

- Adjust the horizontal fold change lines by click-dragging one line or entering a value in the **Fold Change** text box, then clicking **Update**.
- Display labels for data points by clicking a data point.
- Select a gene from the **Up Regulated** or **Down Regulated** list to highlight the corresponding data point in the plot. Press and hold **Ctrl** or **Shift** to select multiple genes.
- Zoom the plot by selecting **Tools > Zoom In** or **Tools > Zoom Out**.
- View lists of significantly up-regulated and down-regulated genes, and optionally, export the gene labels and indices to a structure in the MATLAB workspace by clicking **Export**.
- Normalize the data by clicking the **Normalize** button, then selecting whether to show the normalized plot in a separate window. If you show the normalized plot in a separate window, the **Show smooth curve** check box becomes available in the original (unnormalized) plot.

Note To select different lowess normalization options before normalizing, select **Tools > Set LOWESS Normalization Options**, then select options from the Options dialog box.

Examples

1. Use the `gprread` function to create a structure containing microarray data.

   ```
   maStruct = gprread('mouse_a1wt.gpr');
   ```

2. Use the `magetfield` function to extract the green (cy3) and red (cy5) signals from the structure.

```
cy3data = magetfield(maStruct,'F635 Median');
cy5data = magetfield(maStruct,'F532 Median');
```

3 Create an intensity versus ratio scatter plot of the cy3 and cy5 data. Normalize the data and add a title and labels:

```
mairplot(cy3data, cy5data, 'Normalize', true, ...
    'Title','Normalized R vs G IR plot', ...
    'Labels', maStruct.Names)
```

4 Return intensity values and ratios without displaying the plot.

```
[intensities, ratios] = mairplot(cy3data, cy5data, 'Showplot', false);
```

References

[1] Quackenbush, J. (2002). Microarray Data Normalization and Transformation. Nature Genetics Suppl. *32*, 496–501.

[2] Dudoit, S., Yang, Y.H., Callow, M.J., and Speed, T.P. (2002). Statistical Methods for Identifying Differentially Expressed Genes in Replicated cDNA Microarray Experiments. Statistica Sinica *12*, 111–139.

See Also

Bioinformatics Toolbox functions: `maboxplot`, `magetfield`, `maimage`, `mainvarsetnorm`, `maloglog`, `malowess`, `manorm`, `mattest`, `mavolcanoplot`

Purpose

Create loglog plot of microarray data

Syntax

```
maloglog(X, Y, 'PropertyName', PropertyValue...)
maloglog(..., 'FactorLines', N)
maloglog(..., 'Title', TitleValue)
maloglog(..., 'Labels', LabelsValues)
maloglog(..., 'HandleGraphicsName', HGValue)
H = maloglog(...)
```

Arguments

X	A numeric array of microarray expression values from a single experimental condition.
Y	A numeric array of microarray expression values from a single experimental condition.
N	Property to add two lines to the plot showing a factor of *N* change.
TitleValue	A string to use as the title for the plot.
LabelsValue	A cell array of labels for the data in *X* and *Y*. If you specify *LabelsValue*, then clicking a data point in the plot shows the label corresponding to that point.

Description

`maloglog(X, Y, 'PropertyName', PropertyValue...)` creates a loglog scatter plot of `X` versus `Y`. `X` and `Y` are numeric arrays of microarray expression values from two different experimental conditions.

`maloglog(..., 'FactorLines', N)` adds two lines to the plot showing a factor of *N* change.

`maloglog(..., 'Title', TitleValue)` allows you to specify a title for the plot.

`maloglog(..., 'Labels', LabelsValues)` allows you to specify a cell array of labels for the data. If *LabelsValues* is defined, then clicking a data point in the plot shows the label corresponding to that point.

`maloglog(..., 'HandleGraphicsName', HGValue)` allows you to pass optional Handle Graphics property name/property value pairs to the function.

`H = maloglog(...)` returns the handle to the plot.

Examples

```
maStruct = gprread('mouse_a1wt.gpr');
Red = magetfield(maStruct,'F635 Median');
Green = magetfield(maStruct,'F532 Median');
maloglog(Red,Green,'title','Red vs Green');
% Add factorlines and labels
figure
maloglog(Red,Green,'title','Red vs Green',...
                'FactorLines',2,'LABELS',maStruct.Names);
% Now create a normalized plot
figure
maloglog(manorm(Red),manorm(Green),'title',...
                'Normalized Red vs Green','FactorLines',2,...
                'LABELS',maStruct.Names);
```

See Also

Bioinformatics Toolbox functions `maboxplot`, `magetfield`, `mainvarsetnorm`, `maimage`, `mairplot`, `malowess`, `manorm`, `mattest`, `mavolcanoplot`

MATLAB function `loglog`

Purpose

Smooth microarray data using Lowess method

Syntax

```
YSmooth = malowess(X, Y)
malowess(..., 'PropertyName', PropertyValue,...)
malowess(..., 'Order', OrderValue ...)
malowess(..., 'Robust', RobustValue ...)
malowess(..., 'Span', SpanValue ...)
```

Arguments

X, *Y*	Scatter data.
OrderValue	Property to select the order of the algorithm. Enter either `1` (linear fit) or `2` (quadratic fit). The default order is `1`.
RobustValue	Property to select a robust fit. Enter either `true` or `false`.
SpanValue	Property to specify the window size. The default value is `0.05` (5% of total points in *X*)

Description

`YSmooth = malowess(X, Y)` smooths scatter data (`X`, `Y`) using the Lowess smoothing method. The default window size is 5% of the length of `X`.

`malowess(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`malowess(..., 'Order', OrderValue ...)` chooses the order of the algorithm. Note that Curve Fitting Toolbox refers to Lowess smoothing of order `2` as Loess smoothing.

`malowess(..., 'Robust', RobustValue ...)` uses a robust fit when *RobustValue* is set to `true`. This option can take a long time to calculate.

`malowess(..., 'Span', SpanValue ...)` modifies the window size for the smoothing function. If *SpanValue* is less than `1`, the window size is taken to be a fraction of the number of points in the data. If *SpanValue* is greater than `1`, the window is of size *SpanValue*.

Examples

```
maStruct = gprread('mouse_a1wt.gpr');
cy3data = magetfield(maStruct, 'F635 Median');
cy5data = magetfield(maStruct, 'F532 Median');
[x,y] = mairplot(cy3data, cy5data);
drawnow
ysmooth = malowess(x,y);
hold on;
plot(x, ysmooth, 'rx')
ynorm = y - ysmooth;
```

See Also

Bioinformatics Toolbox functions `affyinvarsetnorm`, `maboxplot`, `magetfield`, `maimage`, `mainvarsetnorm`, `mairplot`, `maloglog`, `manorm`, `quantilenorm`

Statistics Toolbox function `robustfit`

Purpose

Normalize microarray data

Syntax

```
XNorm = manorm(X)
XNorm = manorm(MAStruct, FieldName)
[XNorm, ColVal] = manorm(...)
manorm(..., 'Method', MethodValue)
manorm(..., 'Extra_Args', Extra_ArgsValue)
manorm(..., 'LogData', LogDataValue)
manorm(..., 'Percentile', PercentileValue)
manorm(..., 'Global', GlobalValue),
manorm(..., 'StructureOutput', StructureOutputValue)
manorm(..., 'NewColumnName', NewColumnNameValue)
```

Description

`XNorm = manorm(X)` scales the values in each column of microarray data (`X`) by dividing by the mean column intensity.

- `X` — Microarray data. Enter a vector or matrix.
- `XNorm` — Normalized microarray data.

`XNorm = manorm(MAStruct, FieldName)` scales the data for a field (`FieldName`) for each block or print-tip by dividing each block by the mean column intensity. The output is a matrix with each column corresponding to the normalized data for each block.

- `MAStruct` — Microarray structure.

`[XNorm, ColVal] = manorm(...)` returns the values used to normalize the data.

`manorm(..., 'Method',` *`MethodValue`*`)` allows you to choose the method for scaling or centering the data. *`MethodValue`* can be `'Mean'` (default), `'Median'`, `'STD'` (standard deviation), `'MAD'` (median absolute deviation), or a function handle. If you pass a function handle, then the function should ignore NaNs and must return a single value per column of the input data.

`manorm(..., 'Extra_Args', Extra_ArgsValue)` allows you to pass extra arguments to the function *MethodValue*. *Extra_ArgsValue* must be a cell array.

`manorm(..., 'LogData', LogDataValue)`, when *LogDataValue* is `true`, works with log ratio data in which case the mean (or *MethodValue*) of each column is subtracted from the values in the columns, instead of dividing the column by the normalizing value.

`manorm(..., 'Percentile', PercentileValue)` only uses the percentile (*PercentileValue*) of the data preventing large outliers from skewing the normalization. If *PercentileValue* is a vector containing two values, then the range from the *PercentileValue(1)* percentile to the *PercentileValue(2)* percentile is used. The default value is `100`, that is to use all the data in the data set.

`manorm(..., 'Global', GlobalValue)`, when *GlobalValue* is `true`, normalizes the values in the data set by the global mean (or *MethodValue*) of the data, as opposed to normalizing each column or block of the data independently.

`manorm(..., 'StructureOutput', StructureOutputValue)`, when *StructureOutputValue* is `true`, the input data is a structure returns the input structure with an additional data field for the normalized data.

`manorm(..., 'NewColumnName', NewColumnNameValue)`, when using `StructureOutput`, allows you to specify the name of the column that is appended to the list of `ColumnNames` in the structure. The default behavior is to prefix `'Block Normalized'` to the `FieldName` string.

Examples

```
maStruct = gprread('mouse_a1wt.gpr');
% Extract some data of interest.
Red = magetfield(maStruct,'F635 Median');
Green = magetfield(maStruct,'F532 Median');
% Create a log-log plot.
maloglog(Red,Green,'factorlines',true)
% Center the data.
normRed = manorm(Red);
```

```
normGreen = manorm(Green);
% Create a log-log plot of the centered data.
figure
maloglog(normRed,normGreen,'title','Normalized','factorlines',true)

% Alternatively, you can work directly with the structure
normRedBs = manorm(maStruct,'F635 Median - B635');
normGreenBs = manorm(maStruct,'F532 Median - B532');
% Create a log-log plot of the centered data. This includes some
% zero values so turn off the warning.
figure
w = warning('off','Bioinfo:maloglog:ZeroValues');
warning('off','Bioinfo:maloglog:NegativeValues');
maloglog(normRedBs,normGreenBs,'title',...
                'Normalized Background-Subtracted Median Values',...
                'factorlines',true)
        warning(w);
```

See Also

Bioinformatics Toolbox functions `affyinvarsetnorm`, `maboxplot`, `magetfield`, `mainvarsetnorm`, `mairplot`, `maloglog`, `malowess`, `quantilenorm`, `rmasummary`

mapcaplot

Purpose

Create Principal Component Analysis plot of microarray data

Syntax

```
mapcaplot(Data)
mapcaplot(Data, Label)
```

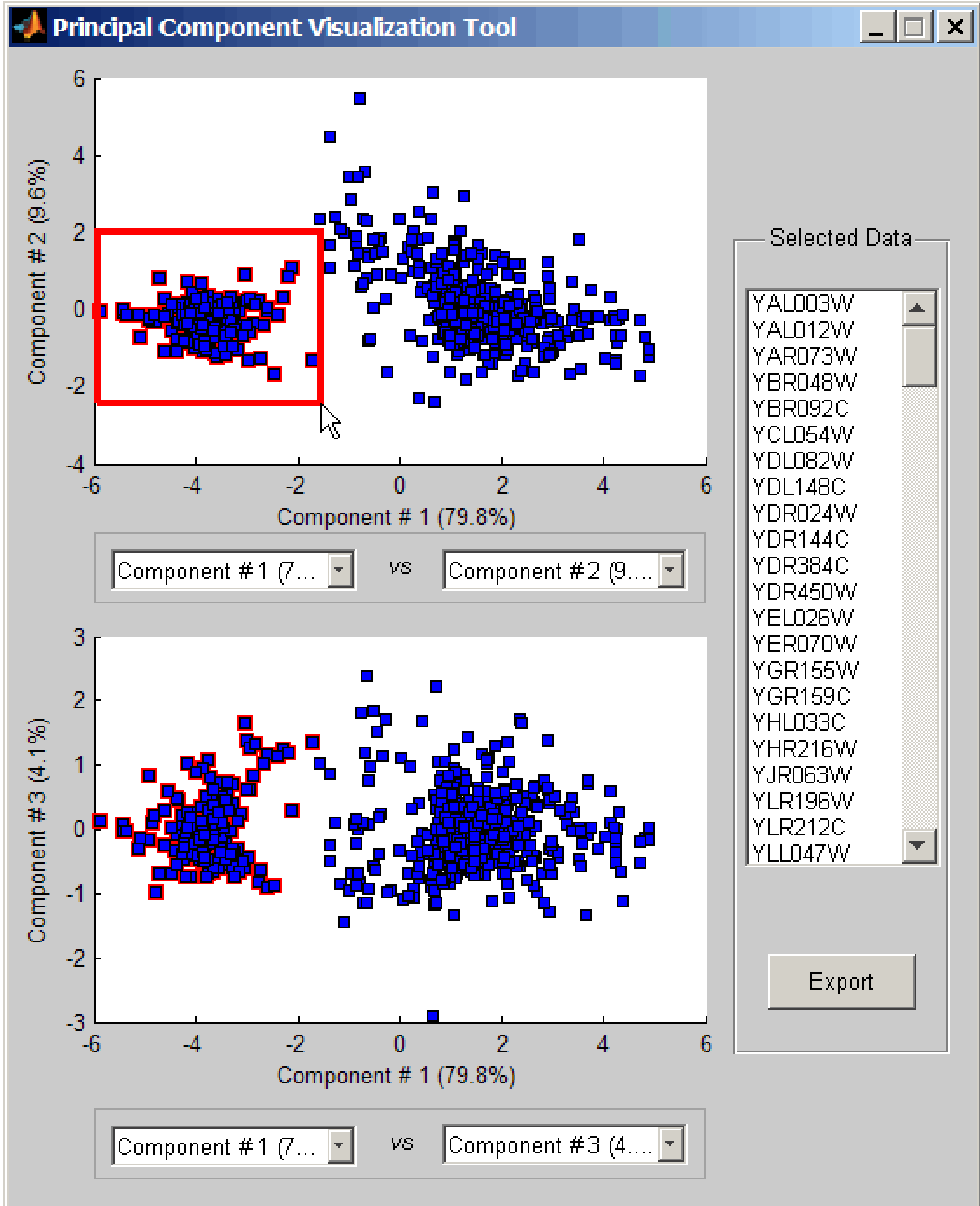
Arguments

Data	Microarray expression profile data.
Label	Cell array of strings representing labels for the data points.

Description

`mapcaplot(`*`Data`*`)` creates 2-D scatter plots of principal components of the array `Data`.

`mapcaplot(`*`Data`*`, `*`Label`*`)` uses the elements of the cell array of strings `Label`, instead of the row numbers, to label the data points.


Principal Component Visualization Tool
Component #2 (9.6%)
Component # 1 (79.8%)
Component #1 (7...
vs
Component #2 (9....
Component #3 (4.1%)
Component # 1 (79.8%)
Component #1 (7...
vs
Component #3 (4....
Selected Data
YAL003W
YAL012W
YAR073W
YBR048W
YBR092C
YCL054W
YDL082W
YDL148C
YDR024W
YDR144C
YDR384C
YDR450W
YEL026W
YER070W
YGR155W
YGR159C
YHL033C
YHR216W
YJR063W
YLR196W
YLR212C
YLL047W
Export

Once you plot the principal components, you can:

- Select principal components for the `x` and `y` axes from the drop-down list boxes below each scatter plot.
- Click a data point to display its label.
- Select a subset of data points by click-dragging a box around them. This will highlight the points in the selected region and the corresponding points in the other axes. The labels of the selected data points appear in the list box.
- Select a label in the list box to highlight the corresponding data point in the plot. Press and hold **Ctrl** or **Shift** to select multiple data points.
- Export the gene labels and indices to a structure in the MATLAB workspace by clicking **Export**.

Examples

```
load filteredyeastdata
mapcaplot(yeastvalues, genes)
```

See Also

Bioinformatics Toolbox functions: `clustergram`, `mattest`, `mavolcanoplot`

Statistics Toolbox function: `princomp`

Purpose

Perform two-tailed t-test to evaluate differential expression of genes from two experimental conditions or phenotypes

Syntax

```
PValues = mattest(DataX, DataY)
[PValues, TScores] = mattest(DataX, DataY)
[PValues, TScores, DFs] = mattest(DataX, DataY)
... = mattest(..., 'Permute', PermuteValue, ...)
... = mattest(..., 'Showhist', ShowhistValue, ...)
... = mattest(..., 'Showplot', ShowplotValue, ...)
... = mattest(..., 'Labels', LabelsValue, ...)
```

Arguments

DataX, *DataY*	Matrices of gene expression values where each row corresponds to a gene and each column corresponds to a replicate. *DataX* and *DataY* must have the same number of rows and are assumed to be normally distributed in each class with equal variances. *DataX* contains data from one experimental condition and *DataY* contains data from a different experimental condition. For example, in a two-color microarray experiment, *DataX* could be cy3 intensity values and *DataY* could be cy5 intensity values.
PermuteValue	Controls whether permutation tests are run, and if so, how many. Choices are `true`, `false` (default), or any integer greater than `2`. If set to `true`, the number of permutations is `1000`.
ShowhistValue	Controls the display of histograms of t-score distributions and p-value distributions. Choices are `true` or `false` (default).

ShowplotValue	Controls the display of a normal t-score quantile plot. Choices are `true` or `false` (default). In the t-score quantile plot, data points with t-scores `> (1 - 1/(2N))` or `< 1/(2N)` display with red circles. `N` is the total number of genes.
LabelsValue	Cell array of labels (typically gene names or probe set IDs) for each row in *DataX* and *DataY*. The labels display if you click a data point in the t-score quantile plot.

Return Values

PValues	Column vector of p-values for each gene in *DataX* and *DataY*.
TScores	Column vector of t-scores for each gene in *DataX* and *DataY*.
DFs	Column vector containing the degree of freedom for each gene in *DataX* and *DataY*.

Description

PValues = `mattest(`*DataX*, *DataY*`)` compares the gene expression profiles in *DataX* and *DataY* and returns a p-value for each gene. *DataX* and *DataY* are matrices of gene expression values, in which each row corresponds to a gene, and each column corresponds to a replicate. *DataX* contains data from one experimental condition and *DataY* contains data from another experimental condition. *DataX* and *DataY* must have the same number of rows and are assumed to be normally distributed in each class with equal variances. *PValues* is a column vector of p-values for each gene.

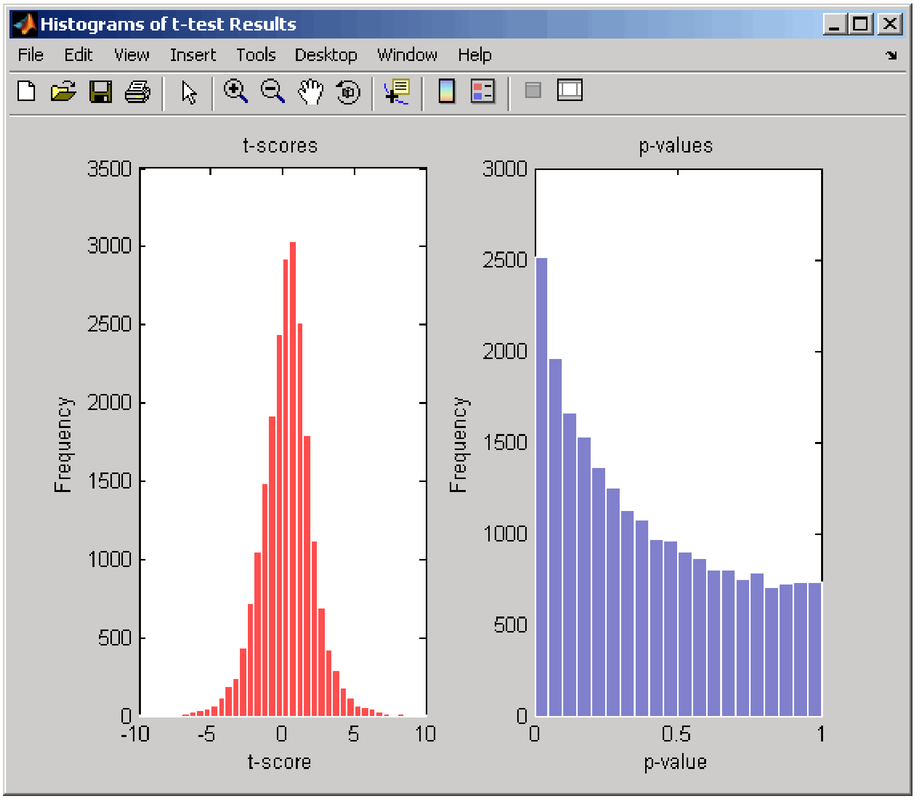
[*PValues*, *TScores*] = `mattest(`*DataX*, *DataY*`)` also returns a t-score for each gene in *DataX* and *DataY*. *TScores* is a column vector of t-scores for each gene.

`[PValues, TScores, DFs] = mattest(DataX, DataY)` also returns *DFs*, a column vector containing the degree of freedom for each gene across both data sets, *DataX* and *DataY*.

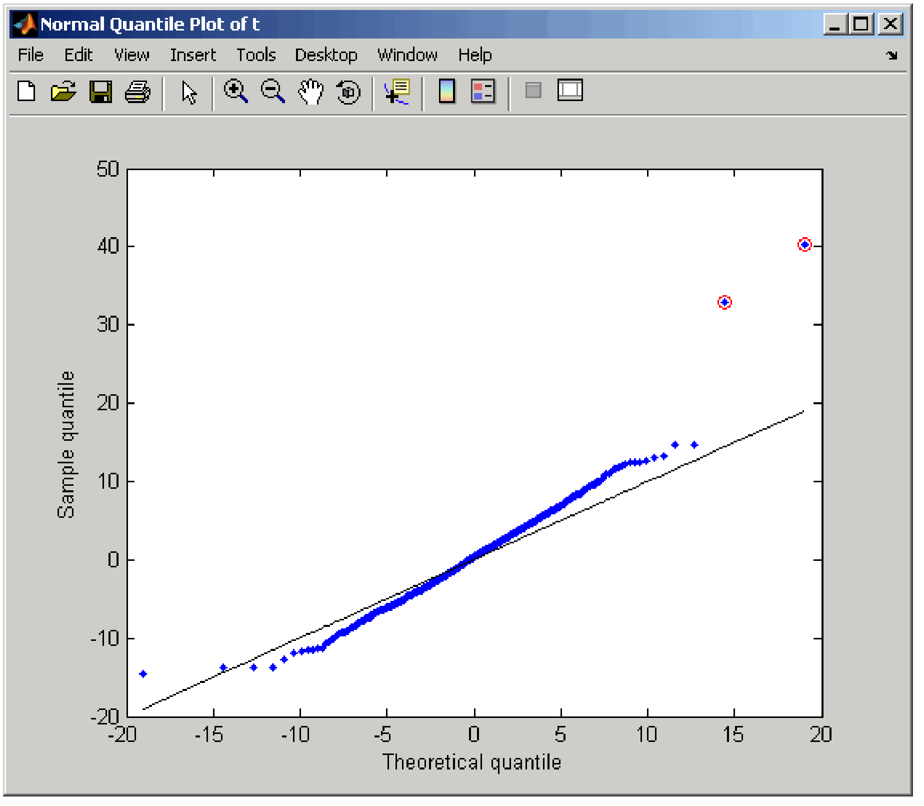
`... = mattest(..., 'PropertyName', PropertyValue, ...)` calls `mattest` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = mattest(..., 'Permute', PermuteValue, ...)` controls whether permutation tests are run, and if so, how many. *PermuteValue* can be `true`, `false` (default), or any integer greater than `2`. If set to `true`, the number of permutations is `1000`.

`... = mattest(..., 'Showhist', ShowhistValue, ...)` controls the display of histograms of t-score distributions and p-value distributions. When *ShowhistValue* is `true`, `mattest` displays histograms. Default is `false`.



`...  = mattest(..., 'Showplot', ShowplotValue, ...)` controls the display of a normal t-score quantile plot. When *`ShowplotValue`* is `true`, `mattest` displays a quantile-quantile plot. Default is `false`. In the t-score quantile plot, the black diagonal line represents the sample quantile being equal to the theoretical quantile. Data points of genes considered to be differentially expressed lie farther away from this line. Specifically, data points with t-scores > `(1 - 1/(2N))` or < `1/(2N)` display with red circles. `N` is the total number of genes.



`...  = mattest(..., 'Labels', LabelsValue, ...)` controls the display of labels when you click a data point in the t-score quantile plot. *`LabelsValue`* is a cell array of labels (typically gene names or probe set IDs) for each row in *`DataX`* and *`DataY`*.

Examples

1 Load the MAT file, included with Bioinformatics Toolbox, that contains Affymetrix data from a prostate cancer study, specifically probe intensity data from Affymetrix HG-U133A GeneChip arrays. The two variables in the MAT file, `dependentData` and `independentData`, are two matrices of gene expression values from two experimental conditions.

```
load prostatecancerexpdata
```

2 Calculate the p-values and t-scores for the gene expression values in the two matrices and display a normal t-score quantile plot.

```
[pvalues,tscores] = mattest(dependentData, independentData,...
                    'showplot',true);
```

3 Calculate the p-values and t-scores again using permutation tests (1000 permutations) and displaying histograms of t-score distributions and p-value distributions.

```
[pvalues,tscores] = mattest(dependentData,independentData,...
                    'permute',true,'showhist',true,...
                    'showplot',true);
```

The `prostatecancerexpdata.mat` file used in this example contains data from Best et al., 2005.

References

[1] Huber, W., von Heydebreck, A., Sültmann, H., Poustka, A., and Vingron, M. (2002). Variance stabilization applied to microarray data calibration and to the quantification of differential expression. Bioinformatics *18 Suppl1*, S96–S104.

[2] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

See Also

Bioinformatics Toolbox functions: `maboxplot`, `mafdr`, `mainvarsetnorm`, `mairplot`, `maloglog`, `malowess`, `manorm`, `mavolcanoplot`, `rmasummary`

Purpose

Create significance versus gene expression ratio (fold change) scatter plot of microarray data

Syntax

```
mavolcanoplot(DataX, DataY, PValues)
SigStructure = mavolcanoplot(DataX, DataY, PValues)
... mavolcanoplot(..., 'Labels', LabelsValue, ...)
... mavolcanoplot(..., 'LogTrans', LogTransValue, ...)
... mavolcanoplot(..., 'PCutoff', PCutoffValue, ...)
... mavolcanoplot(..., 'Foldchange', FoldchangeValue, ...)
```

Arguments

DataX

Matrix or vector of gene expression values from a single experimental condition. If *DataX* is a matrix, each row is a gene, each column is a sample, and an average expression value is calculated for each gene.

Note If the values in *DataX* are natural scale, use the `LogTrans` property to convert them to log 2 scale.

DataY

Matrix or vector of gene expression values from a single experimental condition. If a matrix, each row is a gene, each column is a sample, and an average expression value is calculated for each gene.

Note If the values in *DataY* are natural scale, use the `LogTrans` property to convert them to log 2 scale.

PValues	Vector of p-values for each gene in data sets from two different experimental conditions.
LabelsValue	Cell array of labels (typically gene names or probe set IDs) for the data. After creating the plot, you can click a data point to display the label associated with it. If you do not provide a *LabelsValue*, data points are labeled with row numbers from *DataX* and *DataY*.
LogTransValue	Property to control the conversion of data in *DataX* and *DataY* from natural scale to log 2 scale. Enter `true` to convert data to log 2 scale, or `false`. Default is `false`, which assumes data is already log 2 scale.

PCutoffValue	Lets you specify a cutoff p-value to define data points that are statistically significant. This value is displayed graphically as a horizontal line on the plot. Default is `0.05`, which is equivalent to 1.3010 on the $-\log_{10}$ (p-value) scale. **Note** You can also change the p-value cutoff interactively after creating the plot.
FoldchangeValue	Lets you specify a ratio fold change to define data points that are differentially expressed. Default is `2`, which corresponds to a ratio of 1 and –1 on a $\log_2$ (ratio) scale. **Note** You can also change the fold change interactively after creating the plot.

Description

`mavolcanoplot(`*`DataX, DataY, PValues`*`)` creates a scatter plot of gene expression data, plotting significance versus fold change of gene expression ratios. It uses the average gene expression values from two data sets, *`DataX`* and *`DataY`*, for each gene in the data sets. It plots significance as the $-\log_{10}$ (p-value) from the vector, *`PValues`*. *`DataX`* and *`DataY`* can be vectors or matrices.

`SigStructure` `= mavolcanoplot(`*`DataX, DataY, PValues`*`)` returns a structure containing information for genes that are considered to be both statistically significant (above the p-value cutoff) and significantly differentially expressed (outside of the fold change values). The fields within *`SigStructure`* are sorted by p-value and include:

- `Name`
- `PCutoff`

- `FCThreshold`
- `GeneLabels`
- `PValues`
- `FoldChanges`

`... mavolcanoplot(..., 'PropertyName', PropertyValue, ...)` defines optional properties that use property name/value pairs in any order. These property name/value pairs are as follows:

`... mavolcanoplot(..., 'Labels', LabelsValue, ...)` lets you provide a cell array of labels (typically gene names or probe set IDs) for the data. After creating the plot, you can click a data point to display the label associated with it. If you do not provide a *LabelsValue*, data points are labeled with row numbers from *DataX* and *DataY*.

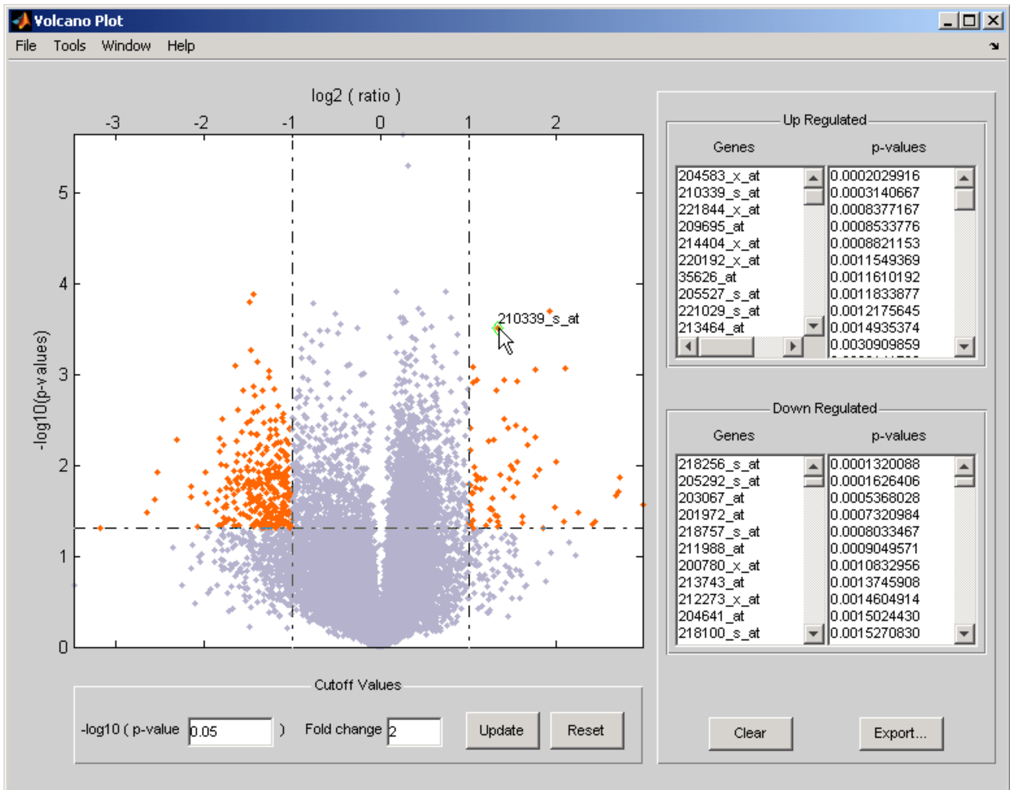
`... mavolcanoplot(..., 'LogTrans', LogTransValue, ...)` controls the conversion of data from *DataX* and *DataY* to $\log_2$ scale. When *LogTransValue* is `true`, `mavolcanoplot` converts data from natural to $\log_2$ scale. Default is `false`, which assumes the data is already $\log_2$ scale.

`... mavolcanoplot(..., 'PCutoff', PCutoffValue, ...)` lets you specify a p-value cutoff to define data points that are statistically significant. This value displays graphically as a horizontal line on the plot. Default is `0.05`, which is equivalent to 1.3010 on the $-\log_{10}$ (p-value) scale.

Note You can also change the p-value cutoff interactively after creating the plot.

`... mavolcanoplot(..., 'Foldchange', FoldchangeValue, ...)` lets you specify a ratio fold change to define data points that are differentially expressed. Fold changes display graphically as two vertical lines on the plot. Default is 2, which corresponds to a ratio of 1 and –1 on a $\log_2$ (ratio) scale.

Note You can also change the fold change interactively after creating the plot.



The volcano plot displays the following:

- $-\log_{10}$ (p-value) versus $\log_2$ (ratio) scatter plot of genes

- Two vertical fold change lines at a fold change level of 2, which corresponds to a ratio of 1 and –1 on a $\log_2$ (ratio) scale. (Lines will be at different fold change levels, if you used the `'Foldchange'` property.)
- One horizontal line at the 0.05 p-value level, which is equivalent to 1.3010 on the $-\log_{10}$ (p-value) scale. (The line will be at a different p-value level, if you used the `'PCutoff'` property.)
- Data points for genes that are considered both statistically significant (above the p-value line) and differentially expressed (outside of the fold changes lines) appear in orange.

After you display the volcano scatter plot, you can interactively:

- Adjust the vertical fold change lines by click-dragging one line or entering a value in the **Fold Change** text box.
- Adjust the horizontal p-value cutoff line by click-dragging or entering a value in the **p-value Cutoff** text box.
- Display labels for data points by clicking a data point.
- Select a gene from the **Up Regulated** or **Down Regulated** list to highlight the corresponding data point in the plot. Press and hold **Ctrl** or **Shift** to select multiple genes.
- Zoom the plot by selecting **Tools > Zoom In** or **Tools > Zoom Out**.
- View lists of significantly up-regulated and down-regulated genes and their associated p-values, and optionally, export the labels, p-values, and fold changes to a structure in the MATLAB Workspace by clicking **Export**.

Examples

1. Load a MAT file, included with Bioinformatics Toolbox, which contains Affymetrix data variables, including `dependentData` and

independentData, two matrices of gene expression values from two experimental conditions.

```
load prostatecancerexpdata
```

2 Use the mattest function to calculate p-values for the gene expression values in the two matrices.

```
pvalues = mattest(dependentData, independentData);
```

3 Using the two matrices, the pvalues calculated by mattest, and the probesetIDs column vector of labels provided, use mavolcanoplot to create a significance versus gene expression ratio scatter plot of the microarray data from the two experimental conditions.

```
mavolcanoplot(dependentData, independentData, pvalues,...
'Labels', probesetIDs)
```

The prostatecancerexpdata.mat file used in the previous example contains data from Best et al., 2005.

References

[1] Cui, X., Churchill, G.A. (2003). Statistical tests for differential expression in cDNA microarray experiments. Genome Biology *4*, 210.

[2] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

See Also

Bioinformatics Toolbox functions: maboxplot, maimage, mainvarsetnorm, mairplot, maloglog, malowess, manorm, mapcaplot, mattest

molweight

Purpose

Calculate molecular weight of amino acid sequence

Syntax

`molweight(SeqAA)`

Arguments

SeqAA	Amino acid sequence. Enter a character string or a vector of integers from the Amino Acid Lookup Table on page 2-42. Examples: `'ARN'`, `[1 2 3]`. You can also enter a structure with the field `Sequence`.

Description

`molweight(SeqAA)` calculates the molecular weight for the amino acid sequence *SeqAA*.

Examples

1 Get an amino acid sequence from the NCBI Genpept Database

```
rhodopsin = getgenpept('NP_000530');
```

2 Calculate the molecular weight of the sequence.

```
rhodopsinMW = molweight(rhodopsin)

rhodopsinMW =

  3.8892e+004
```

See Also

Bioinformatics Toolbox functions: `aacount`, `atomiccomp`, `isoelectric`, `proteinplot`

Purpose Display and manipulate 3-D molecule structure

Syntax

```
molviewer
molviewer(File)
molviewer(pdbID)
molviewer(pdbStruct)
FigureHandle = molviewer(...)
```

Arguments

File

String specifying one of the following:

- File name of a file on the MATLAB search path or in the MATLAB Current Directory
- Path and file name
- URL pointing to a file (URL must begin with a protocol such as http://, ftp://, or file://)

The referenced file is a molecule model file, such as a Protein Data Bank (PDB)-formatted file (ASCII text file). Valid file types include:

- PDB
- MOL (MDL)
- SDF
- XYZ
- SMOL
- JVXL
- CIF/mmCIF

pdbID

String specifying a unique identifier for a protein structure record in the PDB database.

Note Each structure in the PDB database is represented by a four-character alphanumeric identifier. For example, `4hhb` is the identifier for hemoglobin.

---

pdbStruct

A structure containing a field for each PDB record, such as returned by the `getpdb` or `pdbread` function.

Return Values

FigureHandle	Figure handle to a Molecule Viewer window.

Description

`molviewer` opens a blank Molecule Viewer window. You can display 3-D molecular structures by selecting **File > Open**, **File > Load PDB ID**, or **File > Open URL**.

`molviewer(`*`File`*`)` reads the data in a molecule model file, *`File`*, and opens a Molecule Viewer window displaying the 3-D molecular structure for viewing and manipulation.

`molviewer(`*`pdbID`*`)` retrieves the data for a protein structure record, *`pdbID`*, from the PDB database and opens a Molecule Viewer window displaying the 3-D molecular structure for viewing and manipulation.

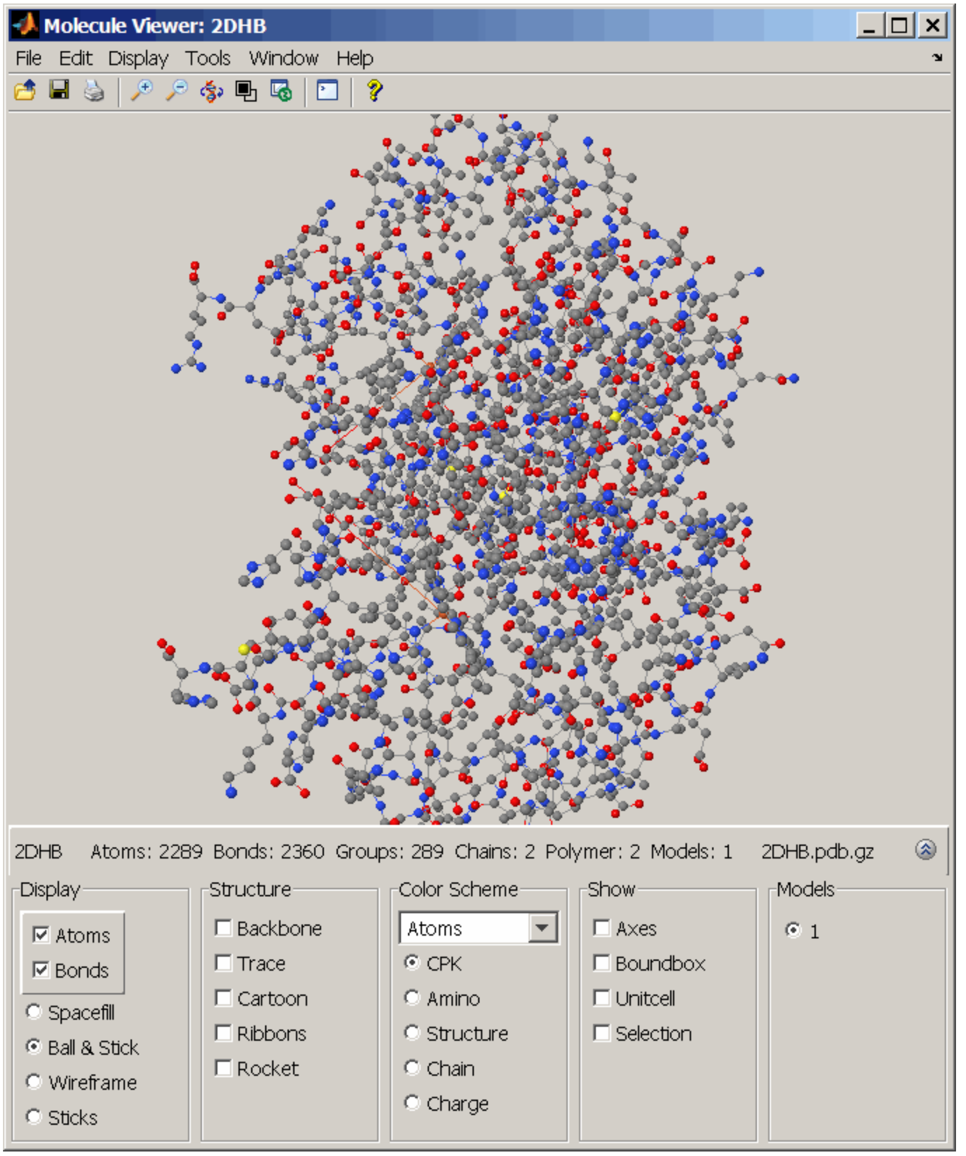
`molviewer(`*`pdbStruct`*`)` reads the data from *`pdbStruct`*, a structure containing a field for each PDB record, and opens a Molecule Viewer window displaying a 3-D molecular structure for viewing and manipulation.

`FigureHandle` `= molviewer(...)` returns the figure handle to the Molecule Viewer window.

Tip You can pass the *`FigureHandle`* to the `evalrasmolscript` function, which sends RasMol script commands to the Molecule Viewer window.

Tip If you receive any errors related to memory or Java heap space, try increasing your Java heap space as described at:

```
http://www.mathworks.com/support/solutions/data/1-18I2C.html
```

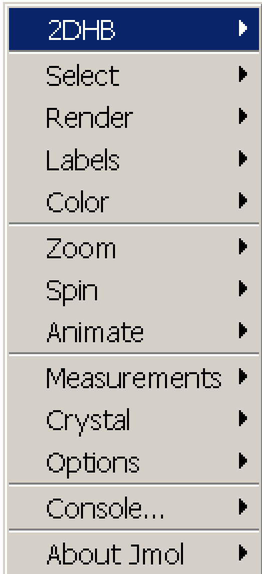

Molecule Viewer: 2DHB
File Edit Display Tools Window Help
2DHB Atoms: 2289 Bonds: 2360 Groups: 289 Chains: 2 Polymer: 2 Models: 1 2DHB.pdb.gz
Display
Atoms
Bonds
Spacefill
Ball & Stick
Wireframe
Sticks
Structure
Backbone
Trace
Cartoon
Ribbons
Rocket
Color Scheme
Atoms
CPK
Amino
Structure
Chain
Charge
Show
Axes
Boundbox
Unitcell
Selection
Models
1

After displaying the 3-D molecule structure, you can:

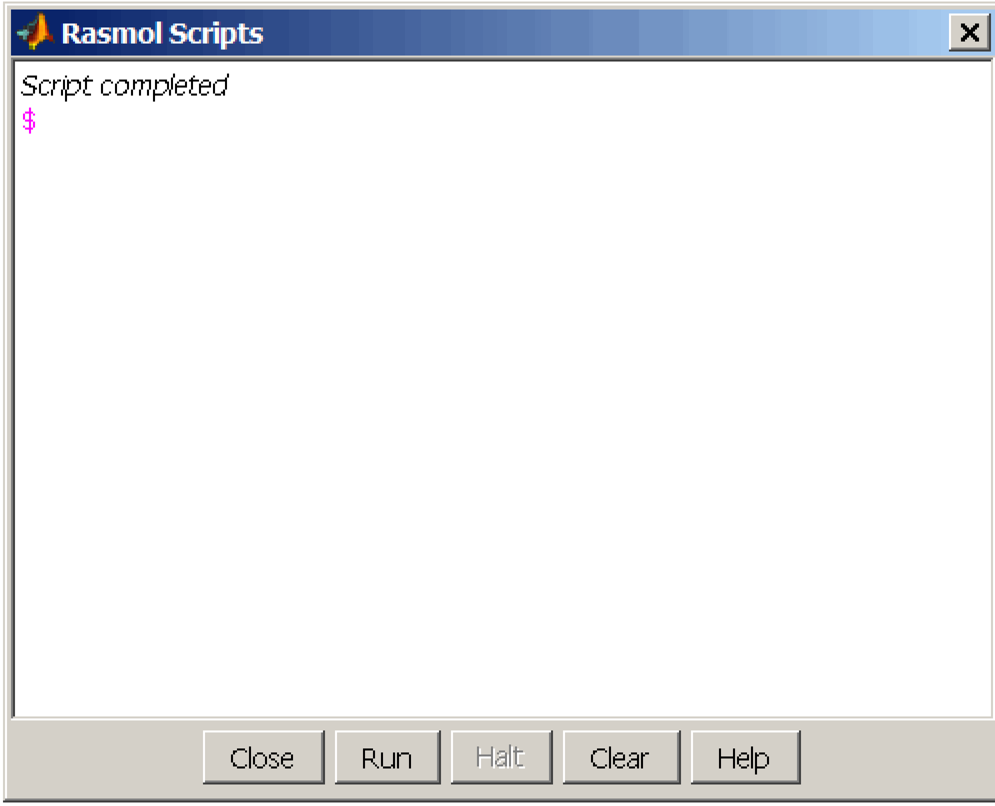
- Click-drag the molecule to spin, rotate, and view it from different angles.
- Hover the mouse over a subcomponent of the molecule to display an identification label for it.
- Zoom the plot by turning the mouse scroll wheel or clicking the following buttons:

   or 

- Spin the molecule by clicking .
- Change the background color between black and white by clicking .
- Reset the molecule position by clicking .
- Show or hide the Control Panel by clicking .
- Manipulate and annotate the 3-D structure by selecting options in the Control Panel or by right-clicking to select commands:



- Display the RasMol Scripts console by clicking .



Examples

View the acetylsalicylic acid (aspirin) molecule, whose structural information is contained in the Elsevier MDL molecule file `aspirin.mol`.

```
molviewer('aspirin.mol')
```

View the H5N1 influenza virus hemagglutinin molecule, whose structural information is located at `www.rcsb.org/pdb/files/2FK0.pdb.gz`.

```
molviewer('http://www.rcsb.org/pdb/files/2FK0.pdb.gz')
```

View the molecule with a PDB identifier of 2DHB.

```
molviewer('2DHB')
```

View the molecule with a PDB identifier of 4hhb, and create a figure handle for the molecule viewer.

```
FH = molviewer('4hhb')
```

Use the getpdb function to retrieve protein structure data from the PDB database and create a MATLAB structure. Then view the protein molecule.

```
pdbstruct = getpdb('1vqx')
molviewer(pdbstruct)
```

See Also

Bioinformatics Toolbox functions: evalrasmolscript, getpdb, pdbread, pdbwrite

Purpose

Align peaks in mass spectrum to reference peaks

Syntax

```
IntensitiesOut = msalign(MZ, Intensities, RefMZ)
... = msalign(..., 'Weights', WeightsValue, ...)
... = msalign(..., 'Range', RangeValue, ...)
... = msalign(..., 'WidthOfPulses',
WidthOfPulsesValue, ...)
... = msalign(..., 'WindowSizeRatio', WindowSizeRatioValue,
   ...)
... = msalign(..., 'Iterations', IterationsValue, ...)
... = msalign(..., 'GridSteps', GridStepsValue, ...)
... = msalign(..., 'SearchSpace', SearchSpaceValue, ...)
... = msalign(..., 'ShowPlot', ShowPlotValue, ...)
[IntensitiesOut, RefMZOut] = msalign(...,
'Group', GroupValue,
   ...)
```

Arguments

MZ — Vector of mass/charge (m/z) values for a spectrum or set of spectra. The number of elements in the vector equals *n* or the number of rows in the matrix *Intensities*.

Intensities — Either of the following:

- Column vector of intensity values for a spectrum, where each row corresponds to an m/z value.
- Matrix of intensity values for a set of mass spectra that share the same m/z range, where each row corresponds to an m/z value, and each column corresponds to a spectrum.

The number of rows equals *n* or the number of elements in vector *MZ*.

RefMZ	Vector of m/z values of known reference masses in a sample spectrum.
	Tip For reference peaks, select compounds that do not undergo structural transformation, such as phosphorylation. Doing so will increase the accuracy of your alignment and allow you to detect compounds that do exhibit structural transformations among the sample spectra.
WeightsValue	Vector of positive values, with the same number of elements as *RefMZ*. The default vector is `ones(size(`*RefMZ*`))`.
RangeValue	Two-element vector, in which the first element is negative and the second element is positive, that specifies the lower and upper limits of a range, in m/z units, relative to each peak. No peak will shift beyond these limits. Default is `[-100 100]`.
WidthOfPulsesValue	Positive value that specifies the width, in m/z units, for all the Gaussian pulses used to build the correlating synthetic spectrum. The point of the peak where the Gaussian pulse reaches `60.65`% of its maximum is set to the width specified by *WidthOfPulsesValue*. Default is `10`.

WindowSizeRatioValue	Positive value that specifies a scaling factor that determines the size of the window around every alignment peak. The synthetic spectrum is compared to the sample spectrum only within these regions, which saves computation time. The size of the window is given in m/z units by *WidthOfPulsesValue* * *WindowSizeRatioValue*. Default is `2.5`, which means at the limits of the window, the Gaussian pulses have a value of `4.39`% of their maximum.
IterationsValue	Positive integer that specifies the number of refining iterations. At every iteration, the search grid is scaled down to improve the estimates. Default is `5`.
GridStepsValue	Positive integer that specifies the number of steps for the search grid. At every iteration, the search area is divided by *GridStepsValue*`^2`. Default is `20`.
SearchSpaceValue	String that specifies the type of search space. Choices are: • `'regular'` — Default. Evenly spaced lattice. • `'latin'` — Random Latin hypercube with *GridStepsValue*`^2` samples.

ShowPlotValue	Controls the display of a plot of an original and aligned spectrum over the reference masses specified by *RefMZ*. Choices are `true`, `false`, or *I*, an integer specifying the index of a spectrum in *Intensities*. If set to `true`, the first spectrum in *Intensities* is plotted. Default is: • `false` — When return values are specified. • `true` — When return values are not specified.
GroupValue	Controls the creation of *RefMZOut*, a new vector of m/z values to be used as reference masses for aligning the peaks. This vector is created by adjusting the values in *RefMZ*, based on the sample data from multiple spectra in *Intensities*, such that the overall shifting and scaling of the peaks is minimized. Choices are `true` or `false` (default). **Tip** Set *GroupValue* to `true` only if *Intensities* contains data for a large number of spectra, and you are not confident of the m/z values used for your reference peaks in *RefMZ*. Leave *GroupValue* set to `false` if you are confident of the m/z values used for your reference peaks in *RefMZ*.

Return Values

IntensitiesOut

Either of the following:

- Column vector intensity values for a spectrum, where each row corresponds to an m/z value.
- Matrix of intensity values for a set of mass spectra that share the same mass/charge (m/z) range, where each row corresponds to an m/z value, and each column corresponds to a spectrum.

The intensity values represent a shifting and scaling of the data.

RefMZOut

Vector of m/z values of reference masses, calculated from *RefMZ* and the sample data from multiple spectra in *Intensities*, when *GroupValue* is set to `true`.

Description

IntensitiesOut = `msalign(`*MZ*, *Intensities*, *RefMZ*`)` aligns the peaks in a raw mass spectrum or spectra, represented by *Intensities* and *MZ*, to reference peaks, provided by *RefMZ*. First, it creates a synthetic spectrum from the reference peaks using Gaussian pulses centered at the m/z values specified by *RefMZ*. Then, it shifts and scales the m/z scale to find the maximum alignment between the input spectrum or spectra and the synthetic spectrum. (It uses an iterative multiresolution grid search until it finds the best scale and shift factors for each spectrum.) Once the new m/z scale is determined, the corrected spectrum or spectra are created by resampling their intensities at the original m/z values, creating *IntensitiesOut*, a vector or matrix of corrected intensity values. The resampling method preserves the shape of the peaks.

Note The `msalign` function works best with three to five reference peaks (marker masses) that you know will appear in the spectrum. If you use a single reference peak (internal standard), there is a possibility of aligning sample peaks to the incorrect reference peaks as `msalign` both scales and shifts the *`MZ`* vector. If using a single reference peak, you might need to only shift the *`MZ`* vector. To do this, use *`IntensitiesOut`* `= interp1(`*`MZ`*`,` *`Intensities`*`,` *`MZ`*`-(`*`ReferenceMass`*`-`*`ExperimentalMass`*`)`. For more information, see Aligning Mass Spectrum with One Reference Peak on page 2-421.

`... = msalign(..., '`*`PropertyName`*`',` *`PropertyValue`*`, ...)` calls `msalign` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = msalign(..., 'Weights',` *`WeightsValue`*`, ...)` specifies the relative weight for each mass in *`RefMZ`*, the vector of reference m/z values. *`WeightsValue`* is a vector of positive values, with the same number of elements as *`RefMZ`*. The default vector is `ones(size(`*`RefMZ`*`))`, which means each reference peak is weighted equally, so that more intense reference peaks have a greater effect in the alignment algorithm. If you have a less intense reference peak, you can increase its weight to emphasize it more in the alignment algorithm.

`... = msalign(..., 'Range',` *`RangeValue`*`, ...)` specifies the lower and upper limits of the range, in m/z units, relative to each peak. No peak will shift beyond these limits. *`RangeValue`* is a two-element vector, in which the first element is negative and the second element is positive. Default is `[-100 100]`.

Note Use these values to tune the robustness of the algorithm. Ideally, you should keep the range within the maximum expected shift. If you try to correct larger shifts by increasing the limits, you increase the possibility of picking incorrect peaks to align to the reference masses.

`... = msalign(..., 'WidthOfPulses', WidthOfPulsesValue, ...)` specifies the width, in m/z units, for all the Gaussian pulses used to build the correlating synthetic spectrum. The point of the peak where the Gaussian pulse reaches `60.65`% of its maximum is set to the width specified by *`WidthOfPulsesValue`*. Choices are any positive value. Default is `10`. *`WidthOfPulsesValue`* may also be a function handle. The function is evaluated at the respective m/z values and returns a variable width for the pulses. Its evaluation should give reasonable values between `0` and `max(abs(Range))`; otherwise, the function returns an error.

Note Tuning the spread of the Gaussian pulses controls a tradeoff between robustness (wider pulses) and precision (narrower pulses). However, the spread of the pulses is unrelated to the shape of the observed peaks in the spectrum. The purpose of the pulse spread is to drive the optimization algorithm.

`... = msalign(..., 'WindowSizeRatio', WindowSizeRatioValue, ...)` specifies a scaling factor that determines the size of the window around every alignment peak. The synthetic spectrum is compared to the sample spectrum only within these regions, which saves computation time. The size of the window is given in m/z units by *`WidthOfPulsesValue * WindowSizeRatioValue`*. Choices are any positive value. Default is `2.5`, which means at the limits of the window, the Gaussian pulses have a value of `4.39`% of their maximum.

`... = msalign(..., 'Iterations', IterationsValue, ...)` specifies the number of refining iterations. At every iteration, the search grid is scaled down to improve the estimates. Choices are any positive integer. Default is `5`.

`... = msalign(..., 'GridSteps', GridStepsValue, ...)` specifies the number of steps for the search grid. At every iteration, the search area is divided by *GridStepsValue*`^2`. Choices are any positive integer. Default is `20`.

`... = msalign(..., 'SearchSpace', SearchSpaceValue, ...)` specifies the type of search space. Choices are:

- `'regular'` — Default. Evenly spaced lattice.
- `'latin'` — Random Latin hypercube with *GridStepsValue*`^2` samples.

`... = msalign(..., 'ShowPlot', ShowPlotValue, ...)` controls the display of a plot of an original and aligned spectrum over the reference masses specified by *RefMZ*. Choices are `true`, `false`, or *I*, an integer specifying the index of a spectrum in *Intensities*. If set to `true`, the first spectrum in *Intensities* is plotted. Default is:

- `false` — When return values are specified.
- `true` — When return values are not specified.

`[IntensitiesOut, RefMZOut] = msalign(..., 'Group', GroupValue, ...)` controls the creation of *RefMZOut*, a new vector of m/z values to be used as reference masses for aligning the peaks. This vector is created by adjusting the values in *RefMZ*, based on the sample data from multiple spectra in *Intensities*, such that the overall shifting and scaling of the peaks is minimized. Choices are `true` or `false` (default).

Tip Set *GroupValue* to `true` only if *Intensities* contains data for a large number of spectra, and you are not confident of the m/z values used for your reference peaks in *RefMZ*. Leave *GroupValue* set to `false` if you are confident of the m/z values used for your reference peaks in *RefMZ*.

Examples

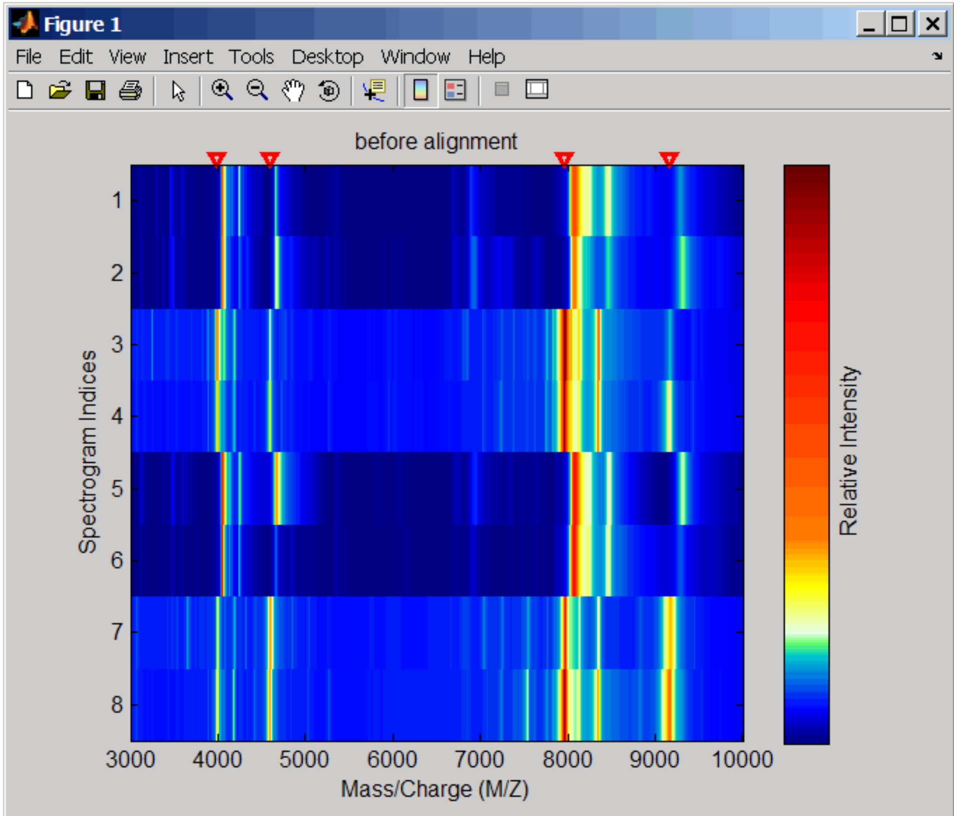
Aligning Mass Spectrum with Three or More Reference Peaks

1 Load sample data, reference masses, and parameter data for synthetic peak width.

```
load sample_lo_res
R = [3991.4 4598 7964 9160];
W = [60 100 60 100];
```

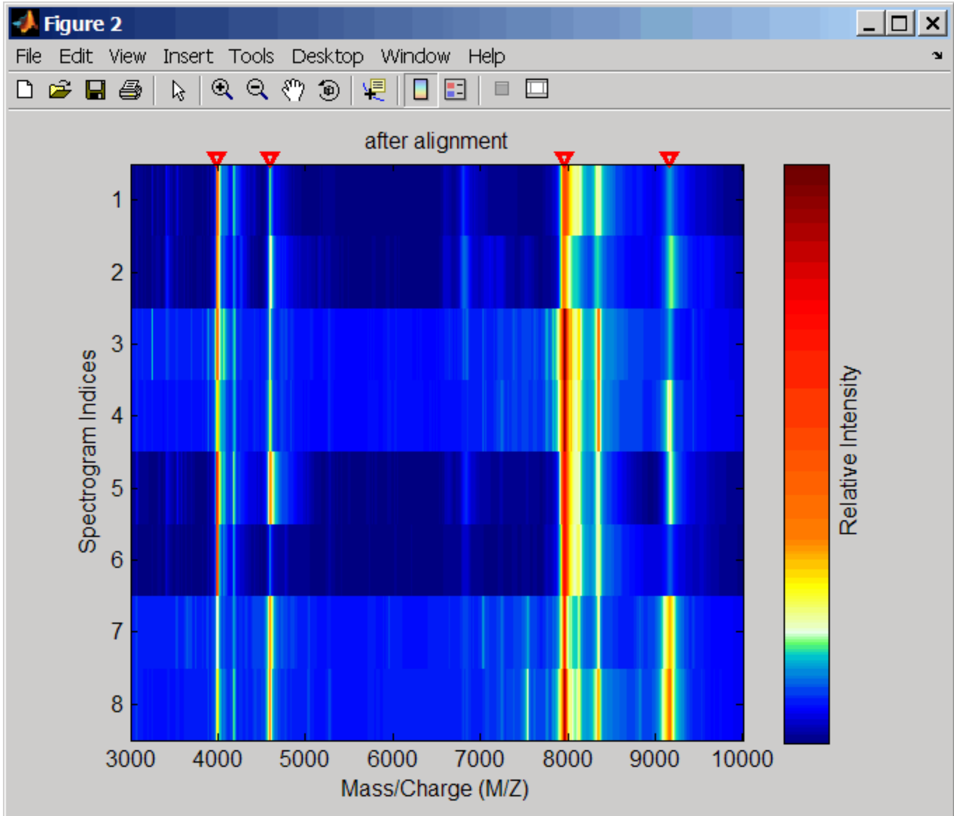
2 Display a color image of the mass spectra before alignment.

```
msheatmap(MZ_lo_res,Y_lo_res,'markers',R,'range',[3000 10000])
title('before alignment')
```



3 Align spectra with reference masses and display a color image of mass spectra after alignment.

```
YA = msalign(MZ_lo_res,Y_lo_res,R,'weights',W);
msheatmap(MZ_lo_res,YA,'markers',R,'range',[3000 10000])
title('after alignment')
```



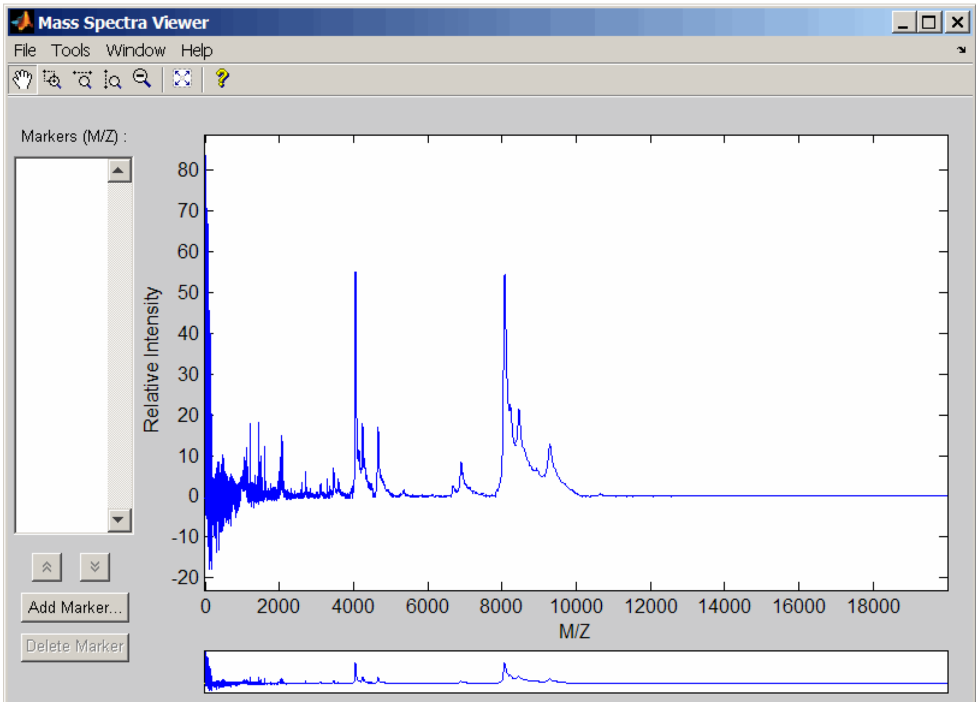
Aligning Mass Spectrum with One Reference Peak

It is not recommended to use the `msalign` function if you have only one reference peak. Instead, use the following procedure, which shifts the *MZ* vector, but does not scale it.

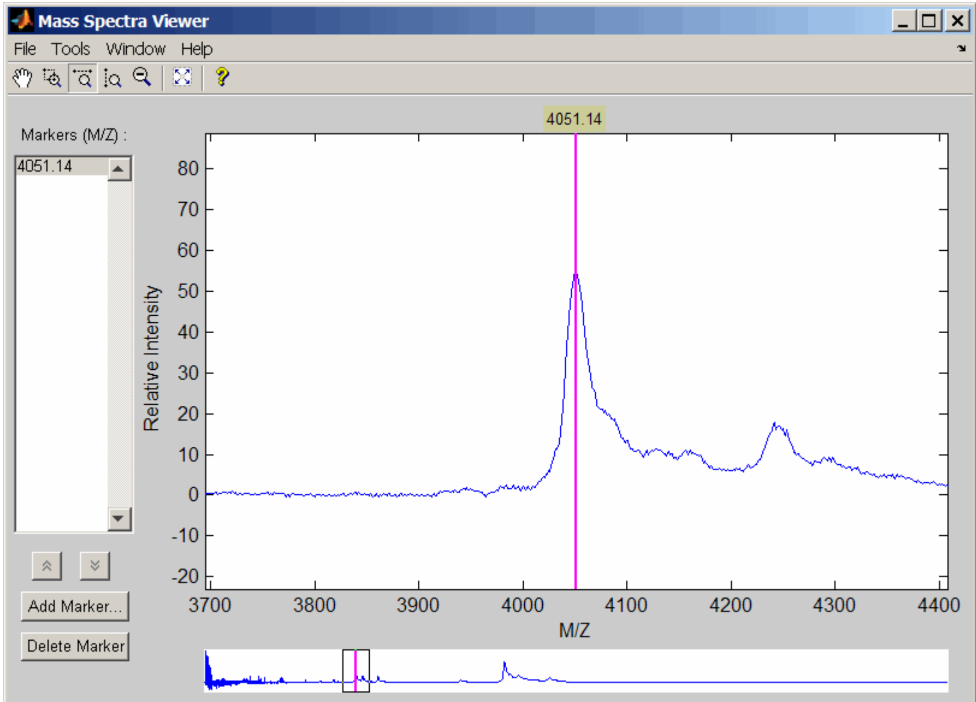
1 Load sample data and view the first sample spectrum.

```
load sample_lo_res
MZ = MZ_lo_res;
Y = Y_lo_res(:,1);
```

```
msviewer(MZ, Y)
```



2 Use the tall peak around 4000 m/z as the reference peak. To determine the reference peak's m/z value, click , and then click-drag to zoom in on the peak. Right-click in the center of the peak, and then click **Add Marker** to label the peak with its m/z value.



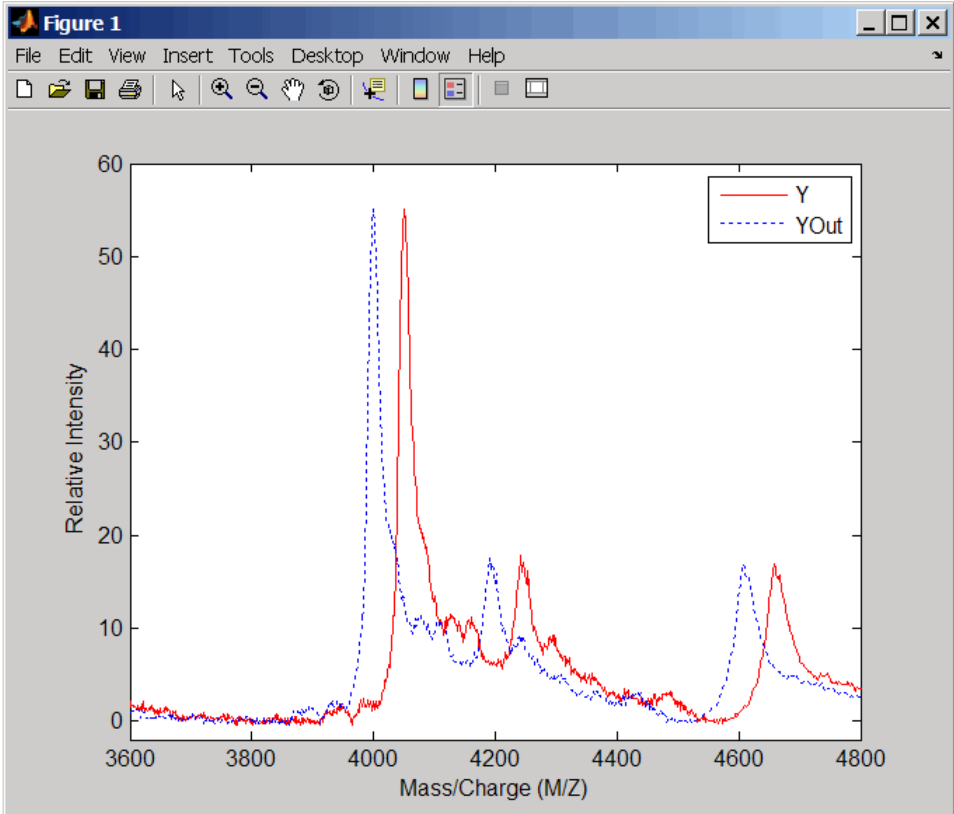
3 Shift a spectrum by the difference between `RP`, the known reference mass of 4000 m/z, and `SP`, the experimental mass of 4051.14 m/z.

```
RP = 4000;
SP = 4051.14;
YOut = interp1(MZ, Y, MZ-(RP-SP));
```

4 Plot the original spectrum in red and the shifted spectrum in blue and zoom in on the reference peak.

```
plot(MZ,Y,'r',MZ,YOut,'b:')
xlabel('Mass/Charge (M/Z)')
ylabel('Relative Intensity')
```

```
legend('Y','YOut')
axis([3600 4800 -2 60])
```



References

[1] Monchamp, P., Andrade-Cetto, L., Zhang, J.Y., and Henson, R. (2007) Signal Processing Methods for Mass Spectrometry. In Systems Bioinformatics: An Engineering Case-Based Approach, G. Alterovitz and M.F. Ramoni, eds. (Artech House Publishers).

See Also

Bioinformatics Toolbox functions: `msbackadj`, `msheatmap`, `mspalign`, `mspeaks`, `msresample`, `msviewer`

Purpose

Correct baseline of mass spectrum

Syntax

```
Yout = msbackadj(MZ, Y)
msbackadj(..., 'PropertyName', PropertyValue,...)
msbackadj(..., 'WindowSize', WindowSizeValue)
msbackadj(..., 'StepSize', StepSizeValue)
msbackadj(..., 'RegressionMethod', RegressionMethodValue)
msbackadj(..., 'EstimationMethod', EstimationMethodValue)
msbackadj(..., 'SmoothMethod', SmoothMethodValue)
msbackadj(..., 'QuantileValue', QuantileValueValue)
msbackadj(..., 'PreserveHeights', PreserveHeightsValue)
msbackadj(..., 'ShowPlot', ShowPlotValue)
```

Arguments

MZ	Range of mass/charge ions. Enter a vector with the range of ions in the spectra.
Y	Ion intensity vector with the same length as the mass/charge vector (*MZ*). *Y* can also be a matrix with several spectra that share the same mass/charge (*MZ*) range.

Description

`Yout = msbackadj(MZ, Y)` adjusts the variable baseline of a raw mass spectrum by following three steps:

1. Estimates the baseline within multiple shifted windows of width 200 m/z
2. Regresses the varying baseline to the window points using a spline approximation
3. Adjusts the baseline of the spectrum (`Y`)

`msbackadj(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`msbackadj(..., 'WindowSize', WindowSizeValue)` specifies the width for the shifting window. *WindowSizeValue* can also be a function handler. The function is evaluated at the respective `MZ` values and returns a variable width for the windows. This option is useful for cases where the resolution of the signal is dissimilar at different regions of the spectrogram. The default value is 200 (baseline point estimated for windows with a width of 200 m/z).

Note The result of this algorithm depends on carefully choosing the window size and the step size. Consider the width of your peaks in the spectrum and the presence of possible drifts. If you have wider peaks towards the end of the spectrum, you may want to use variable parameters.

`msbackadj(..., 'StepSize', StepSizeValue)`specifies the steps for the shifting window. The default value is 200 m/z (baseline point is estimated for windows placed every 200 m/z). *StepSizeValue* may also be a function handle. The function is evaluated at the respective m/z values and returns the distance between adjacent windows.

`msbackadj(..., 'RegressionMethod', RegressionMethodValue)` specifies the method to regress the window estimated points to a soft curve. Enter `'pchip'` (shape-preserving piecewise cubic interpolation), `'linear'`(linear interpolation), or `'spline'`(spline interpolation). The default value is `'pchip'`.

`msbackadj(..., 'EstimationMethod', EstimationMethodValue)` specifies the method for finding the likely baseline value in every window. Enter `'quantile'` (quantile value is set to 10%) or `'em'` (assumes a doubly stochastic model). With `em`, every sample is the independent and identically distributed (i.i.d.) draw of any of two normal distributed classes (background or peaks). Because the class label is hidden, the distributions are estimated with an Expectation-Maximization algorithm. The ultimate baseline value is the mean of the background class.

`msbackadj(..., 'SmoothMethod', SmoothMethodValue)` specifies the method for smoothing the curve of estimated points and eliminating the effects of possible outliers. Enter `'none'`, `'lowess'` (linear fit), `'loess'` (quadratic fit), `'rlowess'` (robust linear), or `'rloess'` (robust quadratic fit). Default value is `'none'`.

`msbackadj(..., 'QuantileValue', QuantileValueValue)` specifies the quantile value. The default value is `0.10`.

`msbackadj(..., 'PreserveHeights', PreserveHeightsValue)`, when *`PreserveHeightsValue`* is `true`, sets the baseline subtraction mode to preserve the height of the tallest peak in the signal. The default value is `false` and peak heights are not preserved.

`msbackadj(..., 'ShowPlot', ShowPlotValue)` plots the baseline estimated points, the regressed baseline, and the original spectrum. When `msbackadj` is called without output arguments, the spectra are plotted unless *`ShowPlotValue`* is `false`. When *`ShowPlotValue`* is `true`, only the first spectrum in `Y` is plotted. *`ShowPlotValue`* can also contain an index to one of the spectra in `Y`.

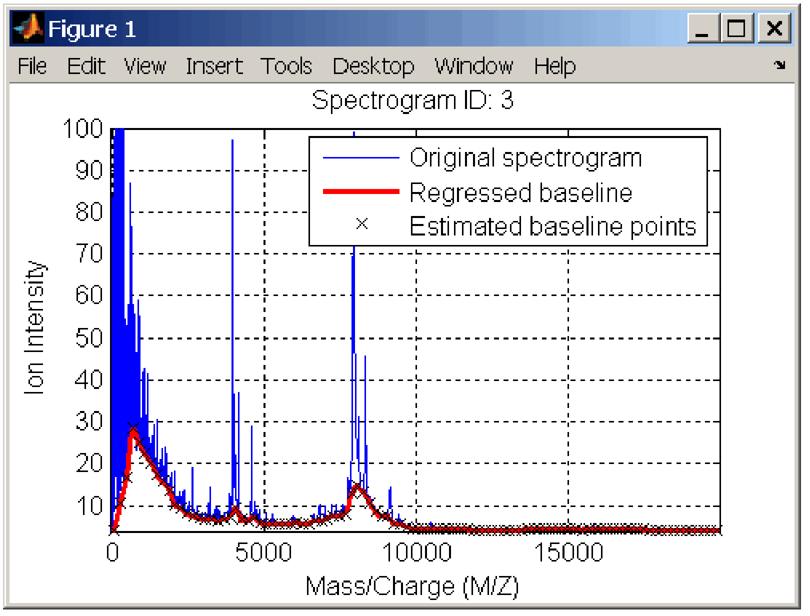
Example

1. Load sample data.

   ```
   load sample_lo_res
   ```

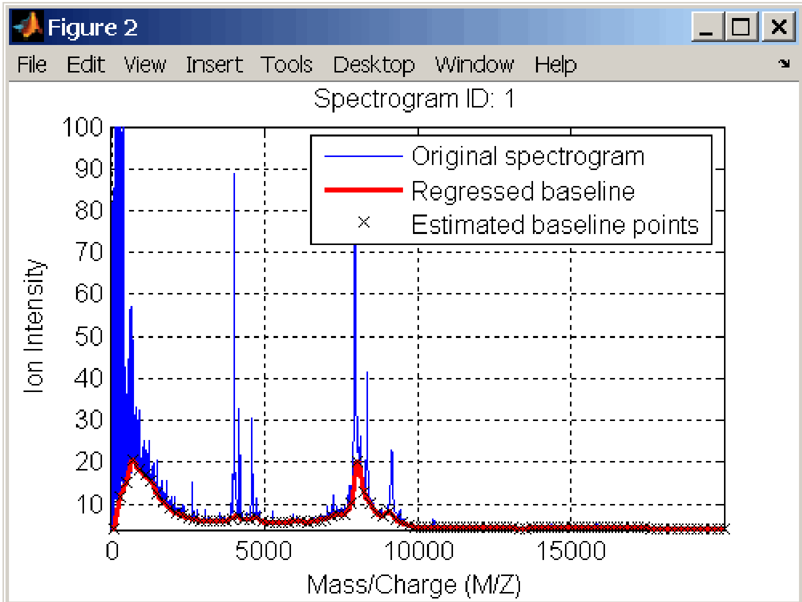
2. Adjust the baseline for a group of spectra and show only the third spectrum and its estimated background.

   ```
   YB = msbackadj(MZ_lo_res,Y_lo_res,'SHOWPLOT',3);
   ```



3 Plot the estimated baseline for the fourth spectrum in `Y_lo_res` using an anonymous function to describe an m/z dependent parameter.

```
wf = @(mz) 200 + .001 .* mz;
msbackadj(MZ_lo_res,Y_lo_res(:,4),'STEPSIZE',wf);
```



See Also

Bioinformatics Toolbox functions `msalign`, `mslowess`, `msheatmap`, `msnorm`, `mspeaks`, `msresample`, `mssgolay`, `msviewer`

msdotplot

Purpose

Plot set of peak lists from LC/MS or GC/MS data set

Syntax

```
msdotplot(Peaks, Times)
msdotplot(FigHandle, Peaks, Times)
msdotplot(..., 'Quantile', QuantileValue)
PlotHandle = msdotplot(...)
```

Arguments

Peaks	Cell array of peak lists, where each element is a two-column matrix with m/z values in the first column and ion intensity values in the second column. Each element corresponds to a spectrum or retention time. **Tip** You can use the `mzxml2peaks` function to create the *Peaks* cell array.
Times	Vector of retention times associated with an LC/MS or GC/MS data set. The number of elements in *Times* equals the number of elements in the cell array *Peaks*. **Tip** You can use the `mzxml2peaks` function to create the *Times* vector.
FigHandle	Handle to an open Figure window such as one created by the `msheatmap` function.
QuantileValue	Value that specifies a percentage. When peaks are ranked by intensity, only those that rank above this percentage are plotted. Choices are any value ≥ `0` and ≤ `1`. Default is `0`. For example, setting *QuantileValue* = `0` plots all peaks, and setting *QuantileValue* = `0.8` plots only the 20% most intense peaks.

Return Values

PlotHandle	Handle to the line series object (figure plot).

Description

`msdotplot(`*`Peaks`*`, `*`Times`*`)` plots a set of peak lists from a liquid chromatography/mass spectrometry (LC/MS) or gas chromatography/mass spectrometry (GC/MS) data set represented by *`Peaks`*, a cell array of peak lists, where each element is a two-column matrix with m/z values in the first column and ion intensity values in the second column, and *`Times`*, a vector of retention times associated with the spectra. *`Peaks`* and *`Times`* have the same number of elements. The data is plotted into any existing figure generated by the `msheatmap` function; otherwise, the data is plotted into a new Figure window.

`msdotplot(`*`FigHandle`*`, `*`Peaks`*`, `*`Times`*`)` plots the set of peak lists into the axes contained in an open Figure window with the handle *`FigHandle`*.

Tip This syntax is useful to overlay a dot plot on top of a heat map of mass spectrometry data created with the `msheatmap` function.

`msdotplot(..., 'Quantile', `*`QuantileValue`*`)` plots only the most intense peaks, specifically those in the percentage above the specified *`QuantileValue`*. Choices are any value ≥ `0` and ≤ `1`. Default is `0`. For example, setting *`QuantileValue`* = `0` plots all peaks, and setting *`QuantileValue`* = `0.8` plots only the 20% most intense peaks.

`PlotHandle`` = msdotplot(...)` returns a handle to the line series object (figure plot). You can use this handle as input to the `get` function to display a list of the plot's properties. You can use this handle as input to the `set` function to change the plot's properties, including showing and hiding points.

Examples

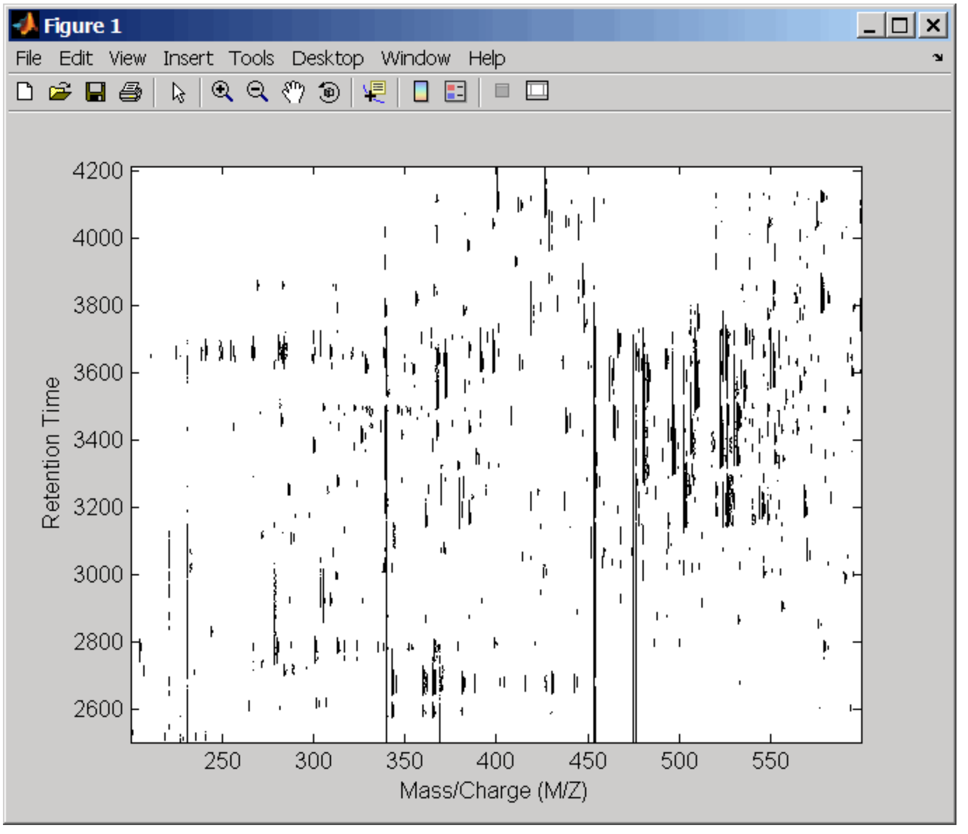
1. Load a MAT file, included with Bioinformatics Toolbox, which contains LC/MS data variables, including `peaks` and `ret_time`. `peaks` is a cell array of peak lists, where each element is a two-column

matrix of m/z values and ion intensity values, and each element corresponds to a spectrum or retention time. `ret_time` is a column vector of retention times associated with the LC/MS data set.

```
load lcmsdata
```

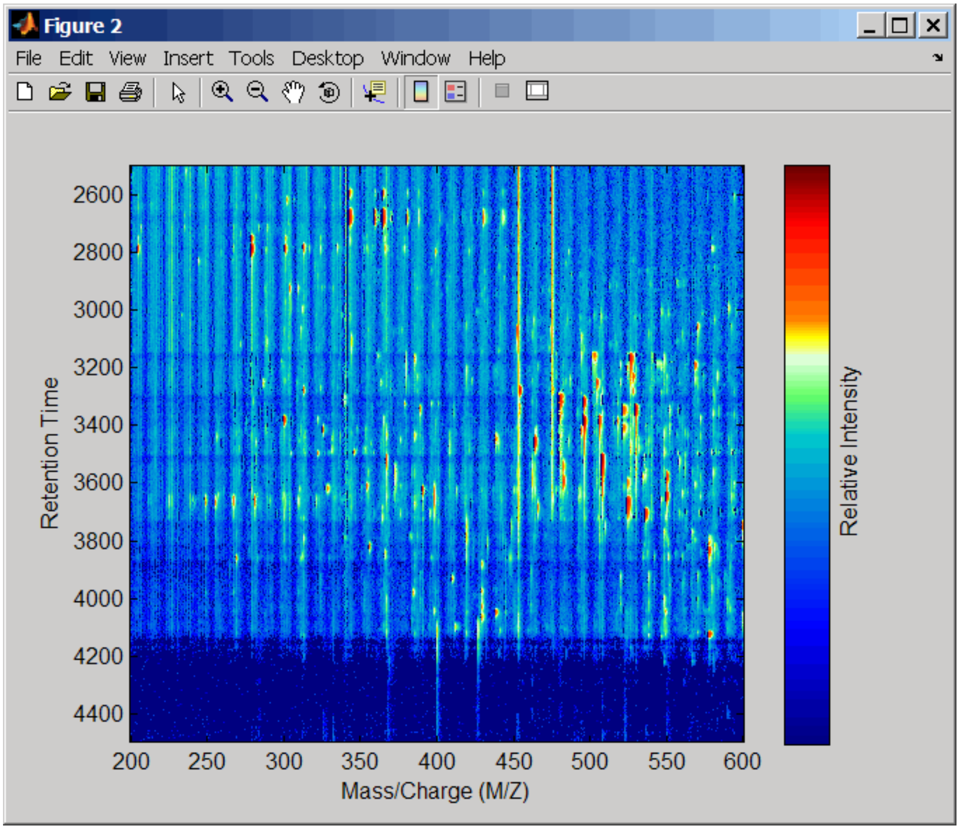
2 Create a dot plot with only the 5% most intense peaks.

```
msdotplot(peaks,ret_time,'Quantile',0.95)
```

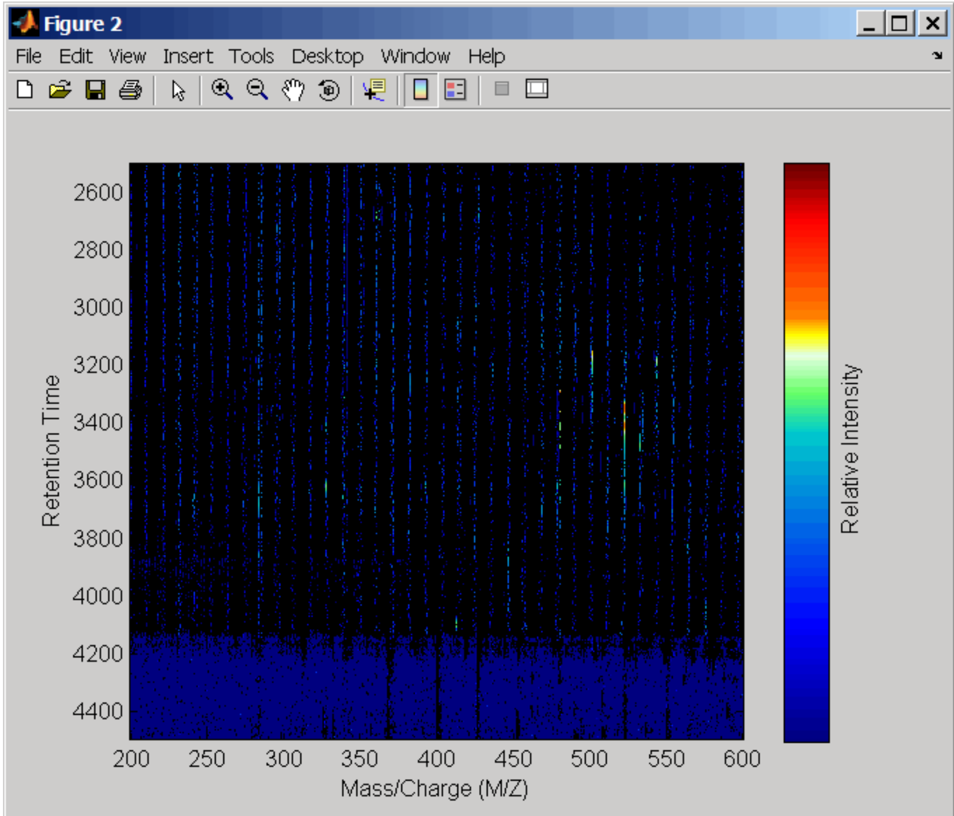


3 Resample the data, then create a heat map and a dot plot of the LC/MS data.

```
[MZ,Y] = msppresample(peaks,5000);
msheatmap(MZ,ret_time,log(Y))
```

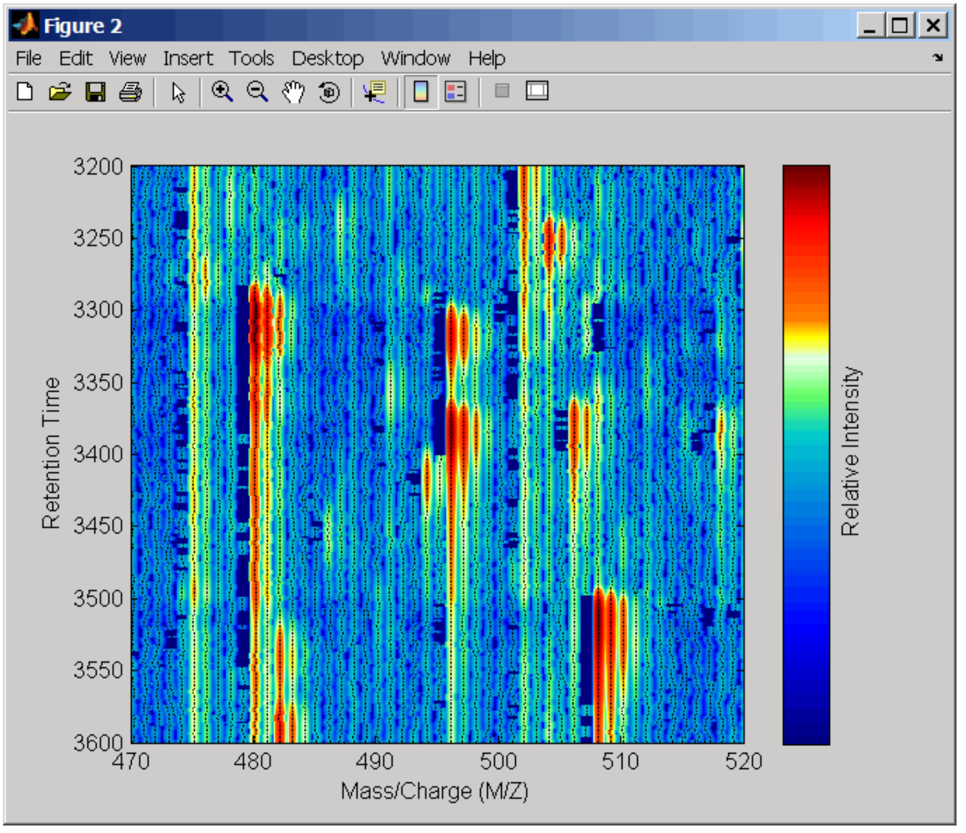



```
msdotplot(peaks,ret_time)
```



4 Zoom in on the heat map to see the detail.

```
axis([470 520 3200 3600])
```



See Also

Bioinformatics Toolbox functions: `msheatmap`, `mspalign`, `mspeaks`, `msppresample`, `mzxml2peaks`, `mzxmlread`

Purpose Create pseudocolor image of set of mass spectra

Syntax

```
msheatmap(MZ, Intensities)
msheatmap(MZ, Times, Intensities)
msheatmap(..., 'Midpoint', MidpointValue, ...)
msheatmap(..., 'Range', RangeValue, ...)
msheatmap(..., 'Markers', MarkersValue, ...)
msheatmap(..., 'SpecIdx', SpecIdxValue, ...)
msheatmap(..., 'Group', GroupValue, ...)
msheatmap(..., 'Resolution', ResolutionValue, ...)
```

Arguments

MZ Column vector of common mass/charge (m/z) values for a set of spectra. The number of elements in the vector equals the number of rows in the matrix *Intensities*.

Note You can use the msppresample function to create the *MZ* vector.

Times Column vector of retention times associated with a liquid chromatography/mass spectrometry (LC/MS) or gas chromatography/mass spectrometry (GC/MS) data set. The number of elements in the vector equals the number of columns in the matrix *Intensities*. The retention times are used to label the *y*-axis of the heat map.

Tip You can use the mzxml2peaks function to create the *Times* vector.

`Intensities` — Matrix of intensity values for a set of mass spectra that share the same m/z range. Each row corresponds to an m/z value, and each column corresponds to a spectrum or retention time. The number of rows equals the number of elements in vector `MZ`. The number of columns equals the number of elements in vector `Times`.

Note You can use the `msppresample` function to create the `Intensities` matrix.

MidpointValue	Value specifying a quantile of the ion intensity values to fall below the midpoint of the color map, meaning they do not represent peaks. `msheatmap` uses a custom color map where cool colors represent nonpeak regions, white represents the midpoint, and warm colors represent peaks. Choices are any value ≥ `0` and ≤ `1`. Default is: • `0.99` — For LC/MS or GC/MS data or when input *T* is provided. This means that 1% of the pixels are warm colors and represent peaks. • `0.95` — For non-LC/MS or non-GC/MS data or when input *T* is not provided. This means that 5% of the pixels are warm colors and represent peaks. **Tip** You can also change the midpoint interactively after creating the heat map by right-clicking the color bar, selecting **Interactive Colormap Shift**, and then click-dragging the cursor vertically on the color bar. This technique is useful when comparing multiple heat maps.
RangeValue	1-by-2 vector specifying the m/z range for the *x*-axis of the heat map. *RangeValue* must be within `[min(`*MZ*`) max(`*MZ*`)]`. Default is the full range `[min(`*MZ*`) max(`*MZ*`)]`.
MarkersValue	Vector of m/z values to mark on the top horizontal axis of the heat map. Default is `[]`.

SpecIdxValue	Either of the following: • Vector of values with the same number of elements as columns (spectra) in the matrix *Intensities*. • Cell array of strings with the same number of elements as columns (spectra) in the matrix *Intensities*. Each value or string specifies a label for the corresponding spectrum. These values or strings are used to label the *y*-axis of the heat map.

Note If input *Times* is provided, it is assumed that *Intensities* contains LC/MS or GC/MS data, and *SpecIdxValue* is ignored.

GroupValue	Either of the following: • Vector of values with the same number of elements as rows in the matrix *Intensities* • Cell array of strings with the same number of elements as rows (spectra) in the matrix *Intensities* Each value or string specifies a group to which the corresponding spectrum belongs. The spectra are sorted and combined into groups along the *y*-axis in the heat map. **Note** If input *Times* is provided, it is assumed that *Intensities* contains LC/MS or GC/MS data, and *GroupValue* is ignored.
ResolutionValue	Value specifying the horizontal resolution of the heat map image. Increase this value to enhance details. Decrease this value to reduce memory usage. Default is: • `0.5` — When *MZ* contains > 2,500 elements. • `0.05` — When *MZ* contains <= 2,500 elements.

Description

`msheatmap(`*`MZ`*`, `*`Intensities`*`)` displays a pseudocolor heat map image of the intensities for the spectra in matrix *Intensities*.

`msheatmap(`*`MZ`*`, `*`Times`*`, `*`Intensities`*`)` displays a pseudocolor heat map image of the intensities for the spectra in matrix *Intensities*, using the retention times in vector *Times* to label the *y*-axis.

`msheatmap(..., '`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `msheatmap` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`msheatmap(..., 'Midpoint', MidpointValue, ...)` specifies a quantile of the ion intensity values to fall below the midpoint of the color map, meaning they do not represent peaks. `msheatmap` uses a custom color map where cool colors represent nonpeak regions, white represents the midpoint, and warm colors represent peaks. Choices are any value between `0` and `1`. Default is:

- `0.99` — For LC/MS or GC/MS data or when input *T* is provided. This means that 1% of the pixels are warm colors and represent peaks.
- `0.95` — For non-LC/MS or non-GC/MS data or when input *T* is not provided. This means that 5% of the pixels are warm colors and represent peaks.

Tip You can also change the midpoint interactively after creating the heat map by right-clicking the color bar, selecting **Interactive Colormap Shift**, then click-dragging the cursor vertically on the color bar. This technique is useful when comparing multiple heat maps.

`msheatmap(..., 'Range', RangeValue, ...)` specifies the m/z range for the *x*-axis of the heat map. *RangeValue* is a 1-by-2 vector that must be within `[min(MZ) max(MZ)]`. Default is the full range `[min(MZ) max(MZ)]`.

`msheatmap(..., 'Markers', MarkersValue, ...)` places markers along the top horizontal axis of the heat map for the m/z values specified in the vector *MarkersValue*. Default is `[]`.

`msheatmap(..., 'SpecIdx', SpecIdxValue, ...)` labels the spectra along the *y*-axis in the heat map. The labels are specified by *SpecIdxValue*, a vector of values or cell array of strings. The number of values or strings is the same as the number of columns (spectra) in the matrix *Intensities*. Each value or string specifies a label for the corresponding spectrum.

`msheatmap(..., 'Group', GroupValue, ...)` sorts and combines spectra into groups along the *y*-axis in the heat map. The groups are specified by *GroupValue*, a vector of values or cell array of strings. The number of values or strings is the same as the number of rows in the matrix *Intensities*. Each value or string specifies a group to which the corresponding spectrum belongs.

`msheatmap(..., 'Resolution', ResolutionValue, ...)` specifies the horizontal resolution of the heat map image. Increase this value to enhance details. Decrease this value to reduce memory usage. Default is:

- 0.5 — When *MZ* contains > 2,500 elements.
- 0.05 — When *MZ* contains <= 2,500 elements.

Examples

SELDI-TOF Data

1 Load SELDI-TOF sample data.

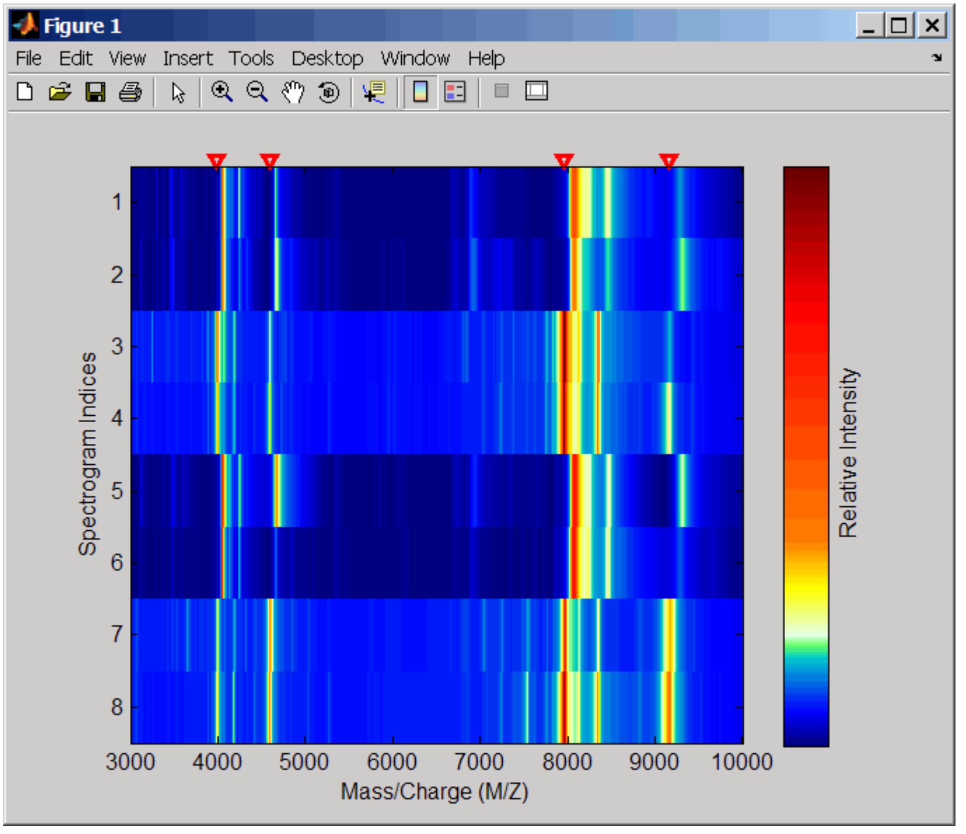
```
load sample_lo_res
```

2 Create a vector of four m/z values to mark along the top horizontal axis of the heat map.

```
M = [3991.4 4598 7964 9160];
```

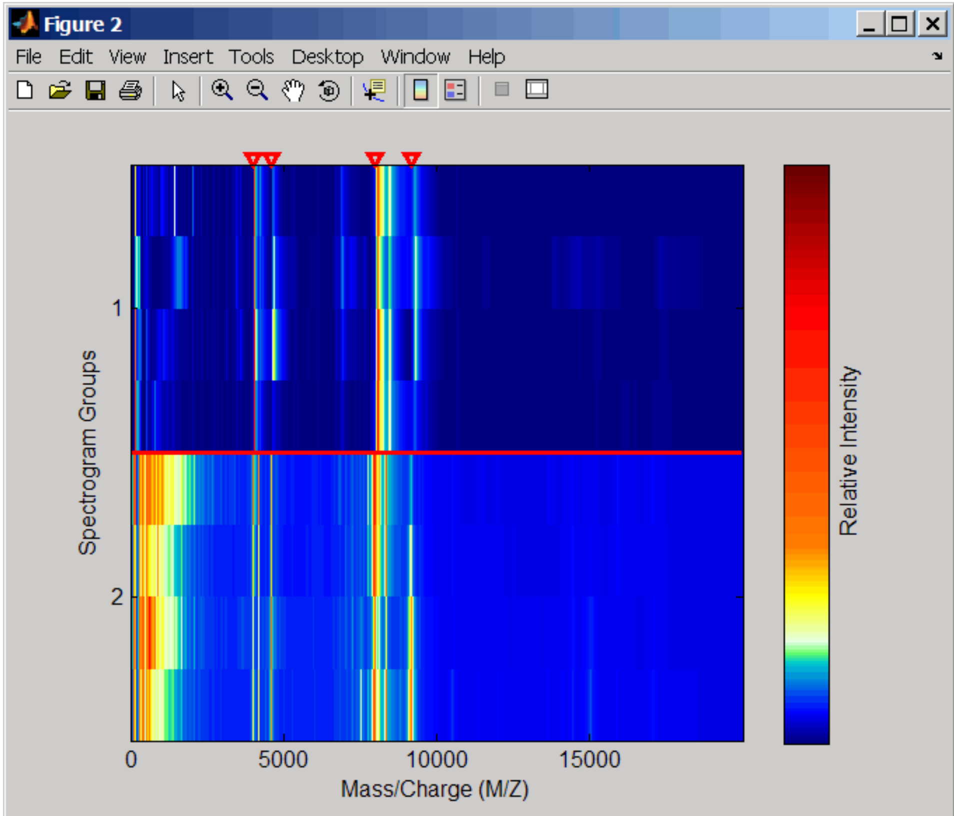
3 Display the heat map with m/z markers and a limited m/z range.

```
msheatmap(MZ_lo_res,Y_lo_res,'markers',M,'range',[3000 10000])
```



4 Display the heat map again grouping each spectrum into one of two groups.

```
TwoGroups = [1 1 2 2 1 1 2 2];
msheatmap(MZ_lo_res,Y_lo_res,'markers',M,'group',TwoGroups)
```



Liquid Chromatography/Mass Spectrometry (LC/MS) Data

1 Load LC/MS sample data.

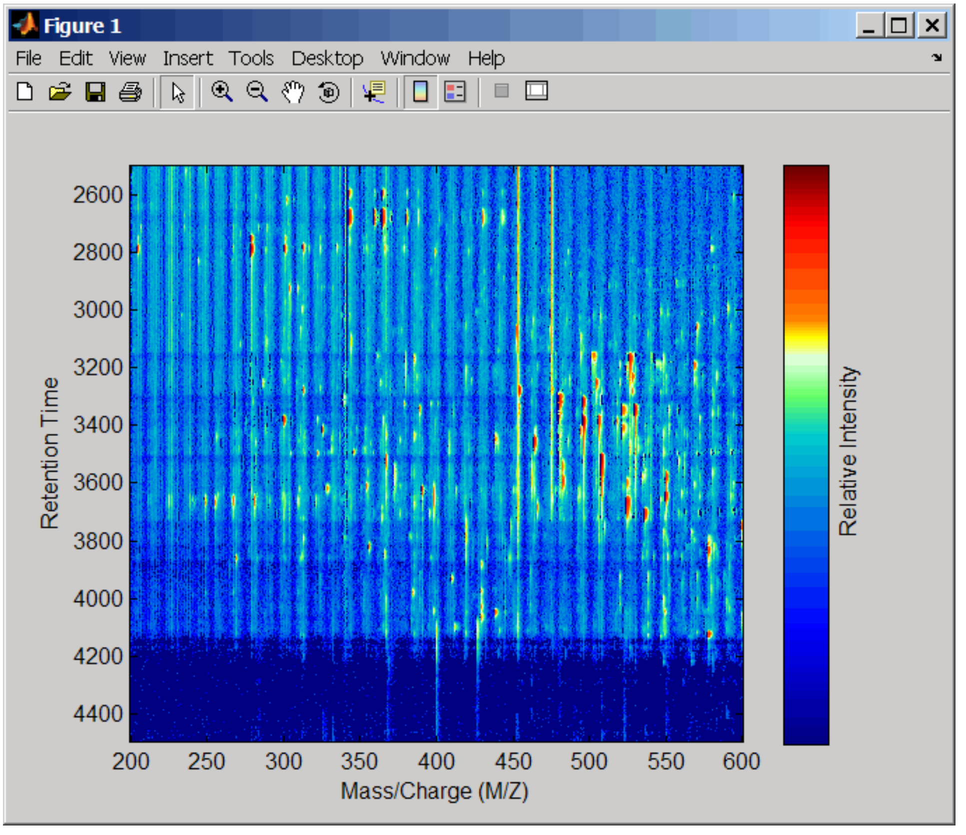
```
load lcmsdata
```

2 Resample the peak lists to create a vector of m/z values and a matrix of intensity values.

```
[MZ, Intensities] = msppresample(peaks, 5000);
```

3 Display the heat map showing mass spectra at different retention times.

```
msheatmap(MZ, ret_time, log(Intensities))
```



See Also

Bioinformatics Toolbox functions: `msalign`, `msbackadj`, `msdotplot`, `mslowess`, `msnorm`, `mspalign`, `msresample`, `mssgolay`, `msviewer`

Purpose

Smooth mass spectrum using nonparametric method

Syntax

```
Yout = mslowess(MZ, Y, 'PropertyName', PropertyValue...)
mslowess(..., 'Order', OrderValue)
mslowess(..., 'Span', SpanValue)
mslowess(..., 'Kernel', KernelValue)
mslowess(..., 'RobustIterations', RobustIterationsValue)
mslowess(..., 'ShowPlot', ShowPlotValue)
```

Arguments

`MZ`	Mass/charge vector with the range of ions in the spectra.
`Y`	Ion intensity vector with the same length as the mass/charge vector (`MZ`). `Y` can also be a matrix with several spectra that share the same mass/charge (`MZ`) range.

Description

`Yout = mslowess(MZ, Y, '`*`PropertyName`*`', `*`PropertyValue`*`...)` smoothes a mass spectrum (`Y`) using a locally weighted linear regression (`lowess`) method with a default span of `10` samples.

Note 1) `mslowess` assumes that a mass/charge vector (`MZ`) might not be uniformly spaced. Therefore, the sliding window for smoothing is centered using the closest samples in terms of the `MZ` value and not in terms of the `MZ` indices.

2) When the vector `MZ` does not have repeated values or NaNs, the algorithm is approximately twice as fast.

`mslowess(..., 'Order', `*`OrderValue`*`)` specifies the order (*`OrderValue`*) of the Lowess smoother. Enter `1` (linear polynomial fit or Lowess), `2` (quadratic polynomial fit or Loess), or `0` (equivalent to a weighted local mean estimator and presumably faster because only a mean computation is performed instead of a least squares regression). The default value is 1.

Note Curve Fitting Toolbox also refers to Lowess smoothing of order 2 as Loess smoothing.

---

mslowess(..., 'Span', *SpanValue*) specifies the window size for the smoothing kernel. If *SpanValue* is greater than 1, the window is equal to *SpanValue* number of samples independent of the mass/charge vector (MZ). The default value is 10 samples. Higher values will smooth the signal more at the expense of computation time. If *SpanValue* is less than 1, the window size is taken to be a fraction of the number of points in the data. For example, when *SpanValue* is 0.005, the window size is equal to 0.50% of the number of points in MZ.

mslowess(..., 'Kernel', *KernelValue*) selects the function (*KernelValue*) for weighting the observed ion intensities. Samples close to the MZ location being smoothed have the most weight in determining the estimate. Enter

```
'tricubic' (default)    (1 - (dist/dmax).^3).^3
'gaussian'              exp(-(2*dist/dmax).^2)
'linear'                1-dist/dmax
```

mslowess(..., 'RobustIterations', *RobustIterationsValue*) specifies the number of iterations (*RobustValue*) for a robust fit. If *RobustIterationsValue* is 0 (default), no robust fit is performed. For robust smoothing, small residual values at every span are outweighed to improve the new estimate. 1 or 2 robust iterations are usually adequate while, larger values might be computationally expensive.

Note For a uniformly spaced `MZ` vector, a nonrobust smoothing with `Order` equal to 0 is equivalent to filtering the signal with the kernel vector.

`mslowess(..., 'ShowPlot', ShowPlotValue)` plots the smoothed spectrum over the original spectrum. When `mslowess` is called without output arguments, the spectra are plotted unless *`ShowPlotValue`* is `false`. When *`ShowPlotValue`* is `true`, only the first spectrum in `Y` is plotted. *`ShowPlotValue`* can also contain an index to one of the spectra in `Y`.

Example

1. Load sample data.

```
load sample_lo_res
```

2. Smooth spectrum and draw figure with unsmoothed and smoothed spectra.

```
YS = mslowess(MZ_lo_res,Y_lo_res(:,1),'Showplot',true);
```

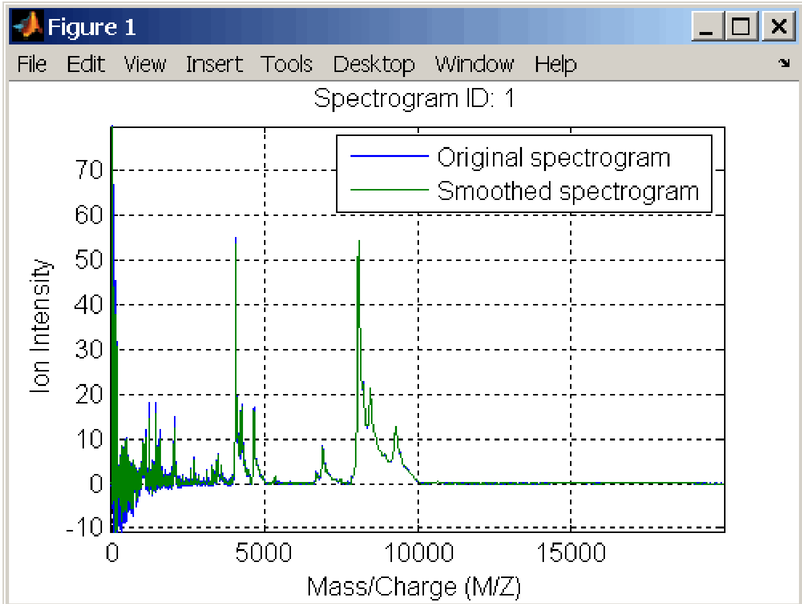
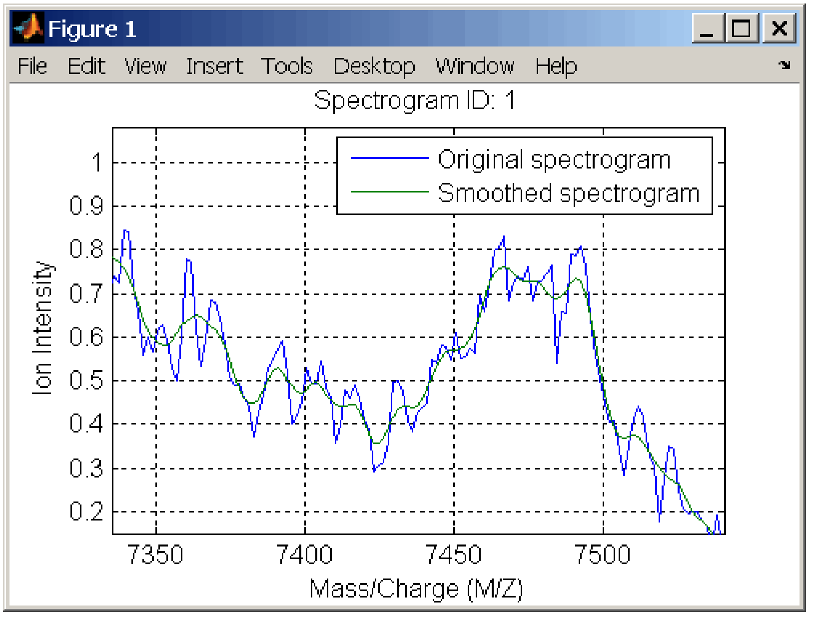


Figure 1
File Edit View Insert Tools Desktop Window Help
Spectrogram ID: 1
Original spectrogram
Smoothed spectrogram
Ion Intensity
70
60
50
40
30
20
10
0
-10
0
5000
10000
15000
Mass/Charge (M/Z)



See Also

Bioinformatics Toolbox functions `msalign`, `msbackadj`, `msheatmap`, `msheatmap`,`msnorm`, `mspeaks`, `msresample`, `mssgolay`, `msviewer`

Purpose

Normalize set of mass spectra

Syntax

```
Yout = msnorm(MZ, Y)
[Yout, NormParameters] = msnorm(...)
msnorm(MZ, NewY, NormParameters)
msnorm(..., 'PropertyName', PropertyValue,...)
msnorm(..., 'Quantile', QuantileValue)
msnorm(..., 'Limits', LimitsValue)
msnorm(..., 'Consensus', ConsensusValue)
msnorm(..., 'Method', MethodValue)
msnorm(..., 'Max', MaxValue)
```

Arguments

MZ	Mass/charge vector with the range of ions in the spectra.
Y	Ion intensity vector with the same length as the mass/charge vector (*MZ*). Y can also be a matrix with several spectra that share the same mass/charge (*MZ*) range.

Description

`Yout = msnorm(MZ, Y)` normalizes a group of mass spectra by standardizing the area under the curve (AUC) to the group median.

`[Yout, NormParameters] = msnorm(...)` returns a structure with the parameters to normalize another group of spectra.

`msnorm(MZ, NewY, NormParameters)` uses the parameter information from a previous normalization (`NormParameters`) to normalize a new set of spectra (`NewY`) with the `MZ` positions and output scale from the previous normalization. `NormParameters` is a structure created by `msnorm`. If a consensus proportion (*ConsensusValue*) was given in the previous normalization, no new `MZ` positions are selected, and normalization is performed using the same `MZ` positions.

`msnorm(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`msnorm(..., 'Quantile', QuantileValue)`specifies a 1-by-2 vector with the quantile limits for reducing the set of `MZ` values. For example, when *`QuantileValue`* is `[0.9 1]`, only the largest `10%` of ion intensities in every spectrum are used to compute the AUC. When *`QuantileValue`* is a scalar, the scalar value represents the lower quantile limit and the upper quantile limit is set to `1`. The default value is `[0 1]` (use the whole area under the curve, AUC).

`msnorm(..., 'Limits', LimitsValue)` specifies a 1-by-2 vector with an `MZ` range for picking normalization points. This parameter is useful to eliminate low-mass noise from the AUC calculation. The default value is `[1, max(MZ)]`.

`msnorm(..., 'Consensus', ConsensusValue)` selects `MZ` positions with a consensus rule to include an `MZ` position into the AUC. Its ion intensity must be within the quantile limits of at least part (*`ConsensusValue`*) of the spectra in `Y`. The same `MZ` positions are used to normalize all the spectrums. Enter a scalar between `0` and `1`.

Use the `Consensus` property to eliminate low-intensity peaks and noise from the normalization.

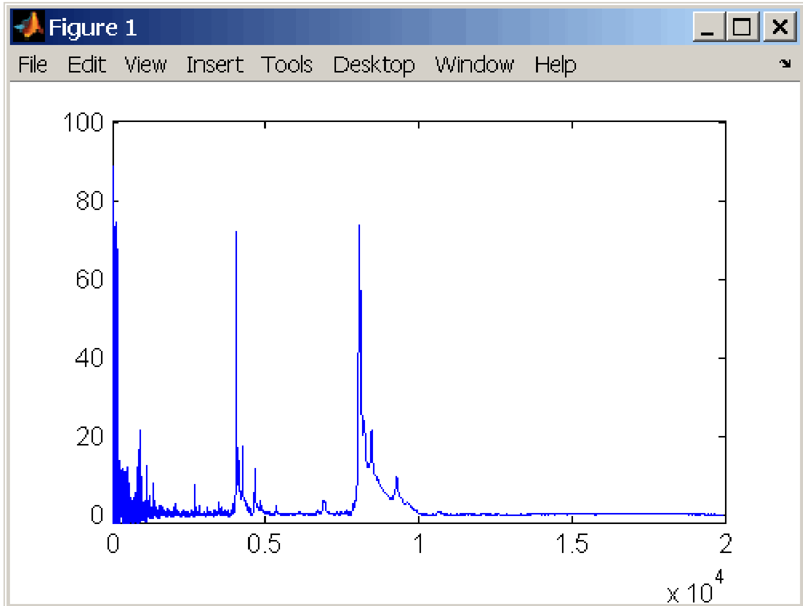
`msnorm(..., 'Method', MethodValue)` selects a method for normalizing the AUC of every spectrum. Enter either `'Median'` (default) or `'Mean'`.

`msnorm(..., 'Max', MaxValue)`, after individually normalizing every spectrum, scales each spectrum to an overall maximum intensity (`Max`). `Max` is a scalar. if omitted, no postscaling is performed. If *`QuantileValue`* is `[1 1]`, then a single point (peak height of the tallest peak) is normalized to `Max`.

Example 1

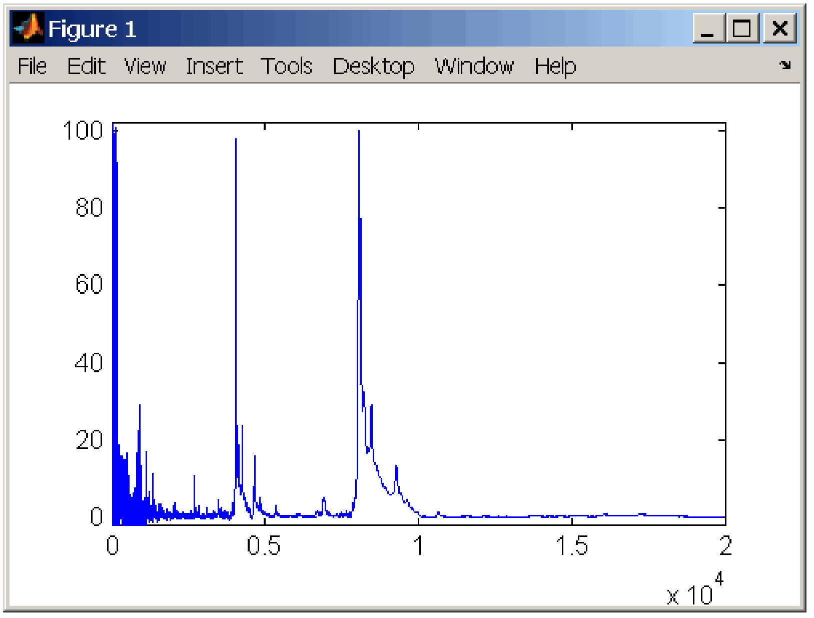
1. Load sample data and plot one of the spectra.

```
load sample_lo_res;
Y = Y_lo_res(:,[1 2 5 6]);
MZ = MZ_lo_res;
plot(MZ, Y(:, 4));
```



2 Normalize the AUC of every spectrum to its median, eliminating low-mass noise, and post-rescaling such that the maximum intensity is 100.

```
Y1 = msnorm(MZ,Y,'Limits',[1000 inf],'Max',100);
plot(MZ, Y1(:, 4));
```



3 Normalize the ion intensity of every spectrum to the maximum intensity of the single highest peak from any of the spectra in the range above 100 m/z.

```
Y2 = msnorm(MZ,Y,'QUANTILE', [1 1],'LIMITS',[1000 inf]);
```

Example 2

1 Select `MZ` regions where the intensities are within the third quartile in at least 90% of the spectrograms.

```
[Y3,S] = msnorm(MZ,Y,'Quantile',[0.5 0.75],'Consensus',0.9);
```

2 Use the same `MZ` regions to normalize another set of spectrograms.

```
Y4 = msnorm(MZ,Y,S);
```

See Also

Bioinformatics Toolbox functions `msalign`, `msbackadj`, `msheatmap`, `mslowess`, `msresample`, `mssgolay`, `msviewer`

Purpose

Align mass spectra from multiple peak lists from LC/MS or GC/MS data set

Syntax

```
[CMZ, AlignedPeaks] = mspalign(Peaks)
[CMZ, AlignedPeaks] = mspalign(Peaks, ...'Quantile',
QuantileValue, ...)
[CMZ, AlignedPeaks] = mspalign(Peaks,
...'EstimationMethod',
   EstimationMethodValue, ...)
[CMZ, AlignedPeaks] = mspalign(Peaks,
...'CorrectionMethod',
   CorrectionMethodValue, ...)
```

Arguments

Peaks	Cell array of peak lists from a liquid chromatography/mass spectrometry (LC/MS) or gas chromatography/mass spectrometry (GC/MS) data set. Each element in the cell array is a two-column matrix with m/z values in the first column and ion intensity values in the second column. Each element corresponds to a spectrum or retention time. **Note** You can use the `mzxml2peaks` function or the `mspeaks` function to create the *Peaks* cell array.
QuantileValue	Value that determines which peaks are selected by the estimation method to create *CMZ*, the vector of common m/z values. Choices are any value ≥ `0` and ≤ `1`. Default is `0.95`.

EstimationMethodValue	String specifying the method to estimate *CMZ*, the vector of common mass/charge (m/z) values. Choices are: • `histogram` — Default method. Peak locations are clustered using a kernel density estimation approach. The peak ion intensity is used as a weighting factor. The center of all the clusters conform to the *CMZ* vector. • `regression` — Takes a sample of the distances between observed significant peaks and regresses the inter-peak distance to create the *CMZ* vector with similar inter-element distances.
CorrectionMethodValue	String specifying the method to align each peak list to the *CMZ* vector. Choices are: • `nearest-neighbor` — Default method. For each common peak in the *CMZ* vector, its counterpart in each peak list is the peak that is closest to the common peak's m/z value. • `shortest-path` — For each common peak in the *CMZ* vector, its counterpart in each peak list is selected using the shortest path algorithm.

Return Values

CMZ	Vector of common mass/charge (m/z) values estimated by the `mspalign` function.
AlignedPeaks	Cell array of peak lists, with the same form as *Peaks*, but with corrected m/z values in the first column of each matrix.

Description

[*CMZ*, *AlignedPeaks*] = mspalign(*Peaks*) aligns mass spectra from multiple peak lists (centroided data), by first estimating *CMZ*, a vector of common mass/charge (m/z) values estimated by considering the peaks in all spectra in *Peaks*, a cell array of peak lists, where each element corresponds to a spectrum or retention time. It then aligns the peaks in each spectrum to the values in *CMZ*, creating *AlignedPeaks*, a cell array of aligned peak lists.

[*CMZ*, *AlignedPeaks*] = mspalign(*Peaks*, ...'*PropertyName*', *PropertyValue*, ...) calls mspalign with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

[*CMZ*, *AlignedPeaks*] = mspalign(*Peaks*, ...'Quantile', *QuantileValue*, ...) determines which peaks are selected by the estimation method to create *CMZ*, the vector of common m/z values. Choices are a scalar between 0 and 1. Default is 0.95.

[*CMZ*, *AlignedPeaks*] = mspalign(*Peaks*, ...'EstimationMethod', *EstimationMethodValue*, ...) specifies the method used to estimate *CMZ*, the vector of common mass/charge (m/z) values. Choices are:

- histogram — Default method. Peak locations are clustered using a kernel density estimation approach. The peak ion intensity is used as a weighting factor. The center of all the clusters conform to the *CMZ* vector.
- regression — Takes a sample of the distances between observed significant peaks and regresses the inter-peak distance to create the *CMZ* vector with similar inter-element distances.

[*CMZ*, *AlignedPeaks*] = mspalign(*Peaks*, ...'CorrectionMethod', *CorrectionMethodValue*, ...) specifies the method used to align each peak list to the *CMZ* vector. Choices are:

- `nearest-neighbor` — Default method. For each common peak in the *CMZ* vector, its counterpart in each peak list is the peak that is closest to the common peak's m/z value.
- `shortest-path` — For each common peak in the *CMZ* vector, its counterpart in each peak list is selected using the shortest path algorithm.

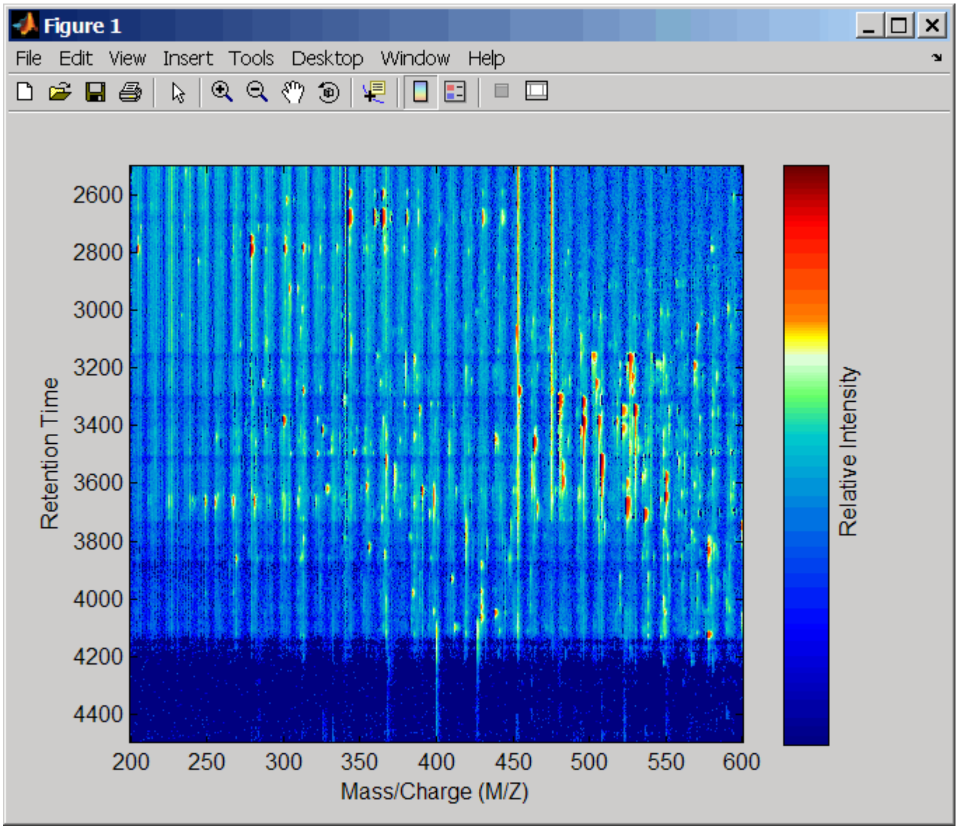
Examples

1. Load a MAT file, included with Bioinformatics Toolbox, which contains liquid chromatography/mass spectrometry (LC/MS) data variables, including `peaks` and `ret_time`. `peaks` is a cell array of peak lists, where each element is a two-column matrix of m/z values and ion intensity values, and each element corresponds to a spectrum or retention time. `ret_time` is a column vector of retention times associated with the LC/MS data set.

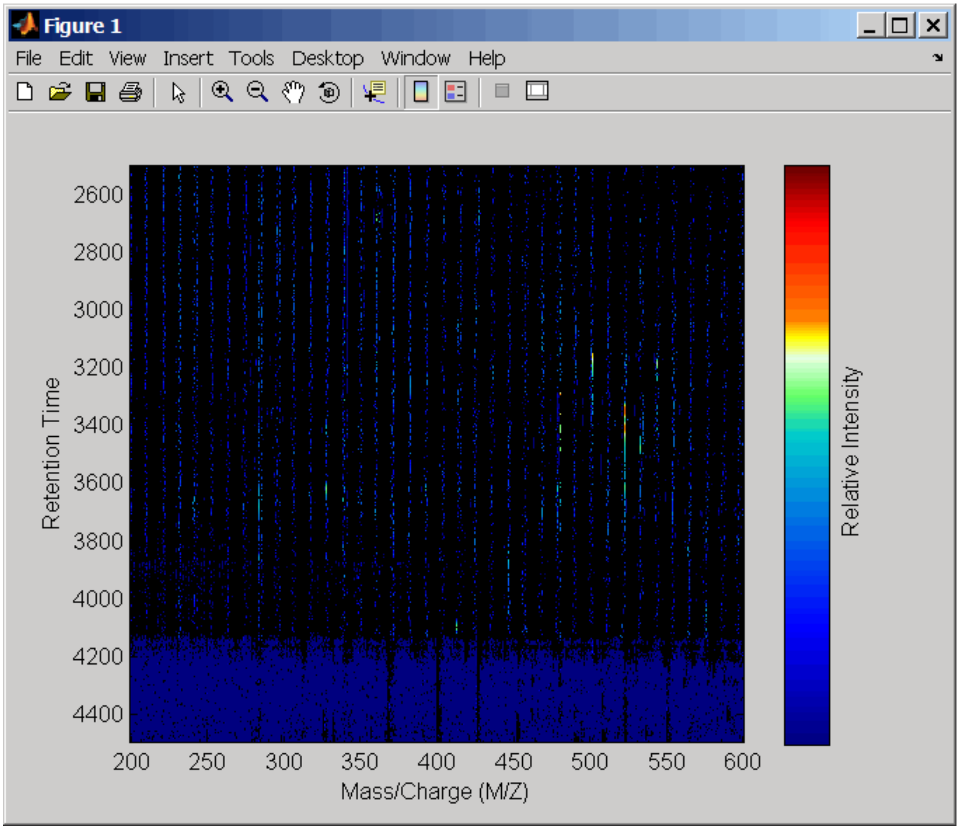
   ```
   load lcmsdata
   ```

2. Resample the unaligned data and display it in a heat map and dot plot.

   ```
   [MZ,Y] = msppresample(peaks,5000);
   msheatmap(MZ,ret_time,log(Y))
   ```




```
msdotplot(peaks,ret_time)
```

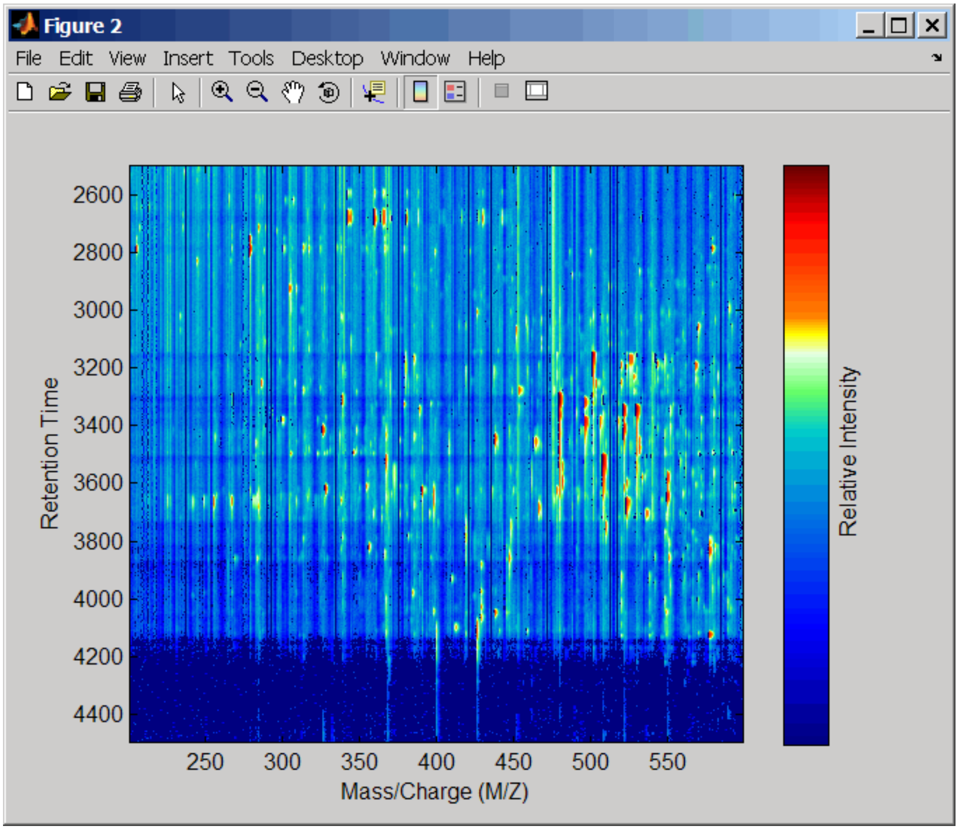


3 Align the peak lists from the mass spectra using the default estimation and correction methods.

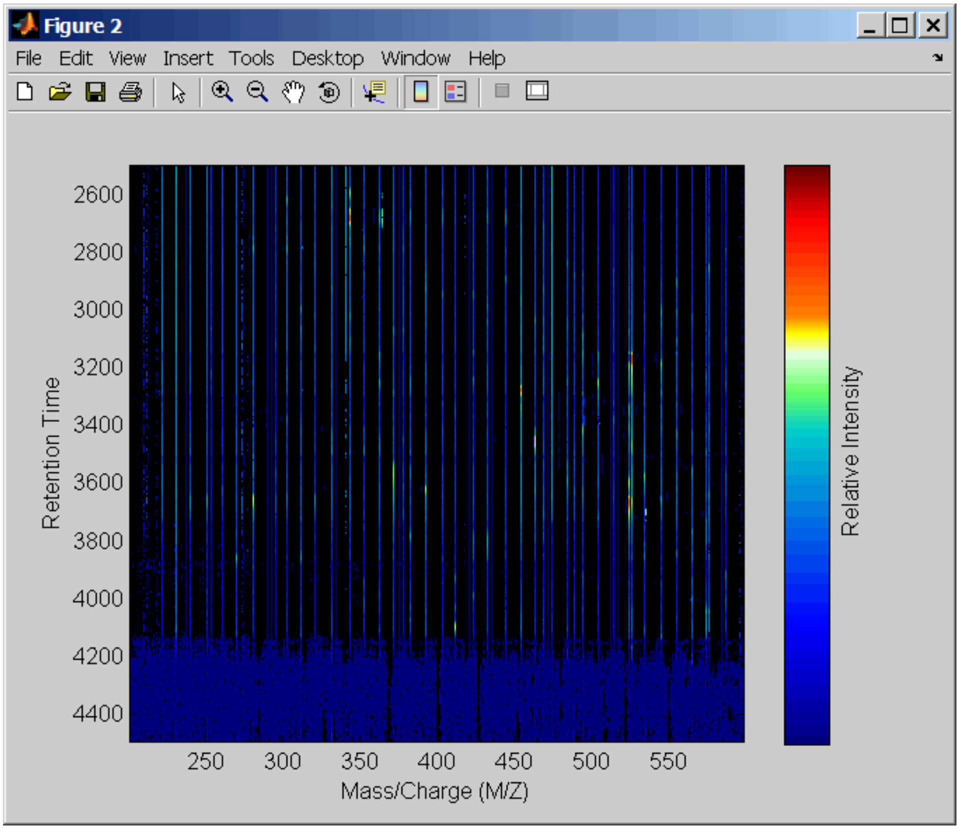
```
[CMZ, aligned_peaks] = mspalign(peaks);
```

4 Resample the unaligned data and display it in a heat map and dot plot.

```
[MZ2,Y2] = msppresample(aligned_peaks,5000);
msheatmap(MZ2,ret_time,log(Y2))
```




```
msdotplot(aligned_peaks,ret_time)
```



5 Link the axes of the two heat plots and zoom in to observe the detail.

```
linkaxes(findobj(0,'Tag','MSHeatMap'))
axis([570 590 3750 3900])
```

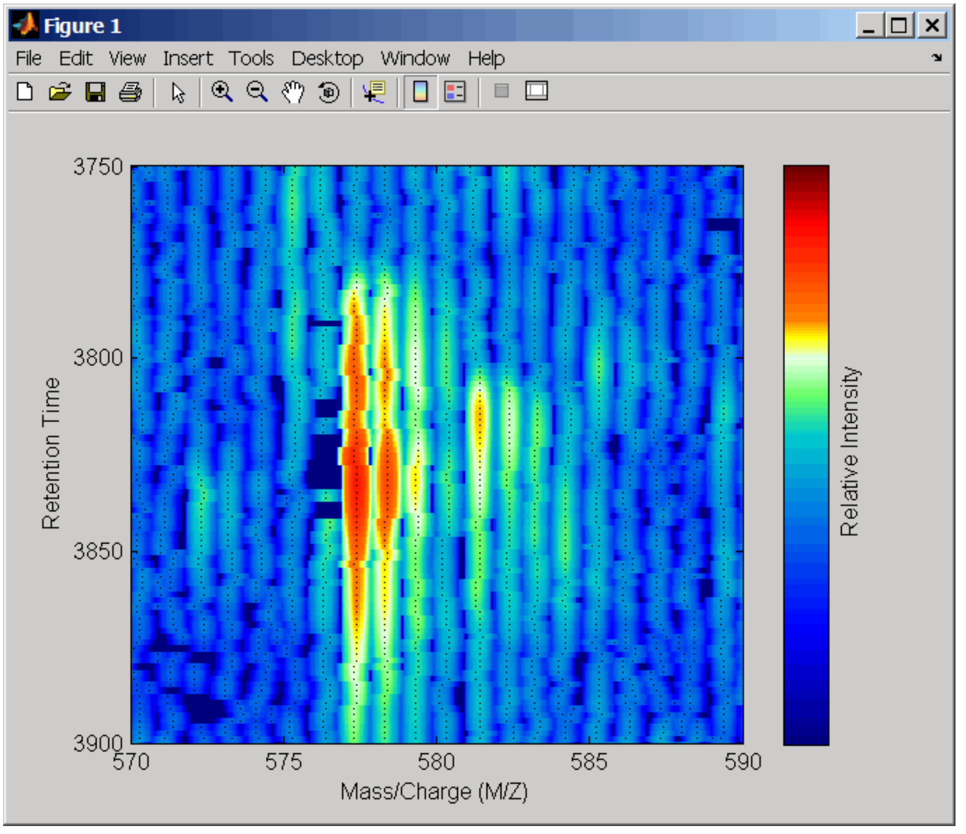
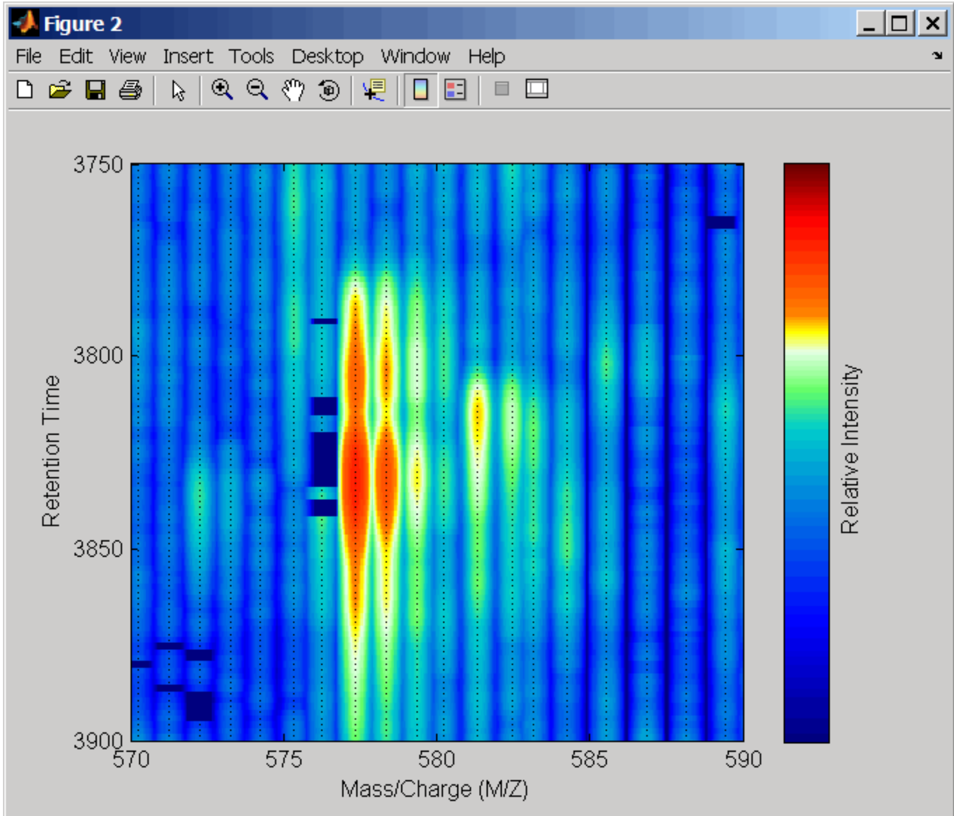


Figure 1
File Edit View Insert Tools Desktop Window Help
3750
3800
3850
3900
570
575
580
585
590
Retention Time
Mass/Charge (M/Z)
Relative Intensity



References

[1] Jeffries, N. (2005) Algorithms for alignment of mass spectrometry proteomic data. Bioinfomatics *21:14*, 3066–3073.

[2] Purvine, S., Kolker, N., and Kolker, E. (2004) Spectral Quality Assessment for High-Throughput Tandem Mass Spectrometry Proteomics. OMICS: A Journal of Integrative Biology *8:3*, 255–265.

See Also

Bioinformatics Toolbox functions: `msalign`, `msdotplot`, `msheatmap`, `mspeaks` , `msppresample`, `mzxml2peaks`

Purpose

Convert raw mass spectrometry data to peak list (centroided data)

Syntax

```
Peaks = mspeaks(MZ, Intensities)
Peaks = mspeaks(MZ, Intensities, ...'Base', BaseValue, ...)
Peaks = mspeaks(MZ, Intensities, ...'Levels', LevelsValue,
   ...)
Peaks = mspeaks(MZ, Intensities, ...'NoiseEstimator',
   NoiseEstimatorValue, ...)
Peaks = mspeaks(MZ, Intensities, ...'Multiplier',
   MultiplierValue, ...)
Peaks = mspeaks(MZ, Intensities, ...'Denoising',
   DenoisingValue, ...)
Peaks = mspeaks(MZ, Intensities, ...'PeakLocation',
   PeakLocationValue, ...)
Peaks = mspeaks(MZ, Intensities, ...'FWHH_Filter',
   FWHH_FilterValue, ...)
Peaks = mspeaks(MZ, Intensities,
...'OverSegmentation_Filter',
   OverSegmentation_FilterValue, ...)
Peaks = mspeaks(MZ, Intensities, ...'Height_Filter',
   Height_FilterValue, ...)
Peaks = mspeaks(MZ, Intensities, ...'ShowPlot',
   ShowPlotValue, ...)
```

Arguments

MZ	Vector of mass/charge (m/z) values for a set of spectra. The number of elements in the vector equals *n* or the number of rows in matrix *Intensities*.
Intensities	Matrix of intensity values for a set of mass spectra that share the same mass/charge (m/z) range. Each row corresponds to an m/z value, and each column corresponds to a spectrum or retention time. The number of rows equals *n* or the number of elements in vector *MZ*.
BaseValue	An integer between 2 and 20 that specifies the wavelet base. Default is 4.
LevelsValue	An integer between 1 and 12 that specifies the number of levels for the wavelet decomposition. Default is 10.

NoiseEstimatorValue	String or scalar that specifies the method to estimate the threshold, `T`, to filter out noisy components in the first high-band decomposition (`y_h`). Choices are: • `mad` — Default. Median absolute deviation, which calculates `T = sqrt(2*log(`*n*`))*mad(`*y_h*`) / 0.6745`, where *n* = the number of rows in the *`Intensities`* matrix. • `std` — Standard deviation, which calculates `T = std(`*y_h*`)`. • A positive real value.
MultiplierValue	A positive real value that specifies the threshold multiplier constant. Default is `1.0`.
DenoisingValue	Controls the use of wavelet denoising to smooth the signal. Choices are `true` (default) or `false`.

Note If your data has previously been smoothed, for example, with the `mslowess` or `mssgolay` function, it is not necessary to use wavelet denoising. Set this property to `false`.

PeakLocationValue	Value that specifies the proportion of the peak height that selects the points used to compute the centroid mass of the respective peak. The value must be ≥ 0 and ≤ 1. Default is 1.0.
FWHH_FilterValue	Positive real value that specifies the minimum full width at half height (FWHH), in m/z units, for reported peaks. Peaks with FWHH below this value are not included in the output list *Peaks*. Default is 0.
OverSegmentation_FilterValue	Positive real value that specifies the minimum distance, in m/z units, between neighboring peaks. When the signal is not smoothed appropriately, multiple maxima can appear to represent the same peak. By increasing this filter value, oversegmented peaks are joined into a single peak. Default is 0.

Height_FilterValue	Positive real value that specifies the minimum height for reported peaks. Default is `0`.
ShowPlotValue	Controls the display of a plot of the original and the smoothed signal, with the peaks included in the output matrix *Peaks* marked. Choices are `true`, `false`, or *I*, an integer specifying the index of a spectrum in *Intensities*. If set to `true`, the first spectrum in *Intensities* is plotted. Default is: • `false` — When return values are specified. • `true` — When return values are not specified.

Return Values

Peaks	Two-column matrix where each row corresponds to a peak. The first column contains mass/charge (m/z) values, and the second column contains ion intensity values.

Description

`Peaks = mspeaks(MZ, Intensities)` finds relevant peaks in raw mass spectrometry data, and creates *Peaks*, a two-column matrix, containing the m/z value and ion intensity for each peak.

`mspeaks` finds peaks by first smoothing the signal using undecimated wavelet transform with Daubechies coefficients, then assigning peak locations, and lastly, eliminating peaks that do not satisfy specified criteria.

`Peaks = mspeaks(MZ, Intensities, ...'PropertyName', PropertyValue, ...)` calls `mspeaks` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`Peaks = mspeaks(MZ, Intensities, ...'Base', BaseValue, ...)` specifies the wavelet base. `BaseValue` must be an integer between `2` and `20`. Default is `4`.

`Peaks = mspeaks(MZ, Intensities, ...'Levels', LevelsValue, ...)` specifies the number of levels for the wavelet decomposition. `LevelsValue` must be an integer between `1` and `12`. Default is `10`.

`Peaks = mspeaks(MZ, Intensities, ...'NoiseEstimator', NoiseEstimatorValue, ...)` specifies the method to estimate the threshold, T, to filter out noisy components in the first high-band decomposition (`y_h`). Choices are:

- `mad` — Default. Median absolute deviation, which calculates `T = sqrt(2*log(n))*mad(y_h) / 0.6745`, where *n* = the number of rows in the `Intensities` matrix.
- `std` — Standard deviation, which calculates `T = std(y_h)`.
- A positive real value.

`Peaks = mspeaks(MZ, Intensities, ...'Multiplier', MultiplierValue, ...)` specifies the threshold multiplier constant. `MultiplierValue` must be a positive real value. Default is `1.0`.

`Peaks = mspeaks(MZ, Intensities, ...'Denoising', DenoisingValue, ...)` controls the use of wavelet denoising to smooth the signal. Choices are `true` (default) or `false`.

Note If your data has previously been smoothed, for example, with the `mslowess` or `mssgolay` function, it is not necessary to use wavelet denoising. Set this property to `false`.

`*Peaks* = mspeaks(*MZ*, *Intensities*, ...'PeakLocation', *PeakLocationValue*, ...)` specifies the proportion of the peak height that selects the points used to compute the centroid mass of the respective peak. *PeakLocationValue* must be a value ≥ `0` and ≤ `1`. Default is `1.0`.

Note When *PeakLocationValue* = `1.0`, the peak location is exactly at the maximum of the peak, while when *PeakLocationValue* = `0`, the peak location is computed with all the points from the closest minimum to the left of the peak to the closest minimum to the right of the peak.

`*Peaks* = mspeaks(*MZ*, *Intensities*, ...'FWHH_Filter', *FWHH_FilterValue*, ...)` specifies the minimum full width at half height (FWHH), in m/z units, for reported peaks. Peaks with FWHH below this value are not included in the output list *Peaks*. *FWHH_FilterValue* must be a positive real value. Default is `0`.

`*Peaks* = mspeaks(*MZ*, *Intensities*, ...'OverSegmentation_Filter', *OverSegmentation_FilterValue*, ...)` specifies the minimum distance, in m/z units, between neighboring peaks. When the signal is not smoothed appropriately, multiple maxima can appear to represent the same peak. By increasing this filter value, oversegmented peaks are joined into a single peak. *OverSegmentation_FilterValue* must be a positive real value. Default is `0`.

`*Peaks* = mspeaks(*MZ*, *Intensities*, ...'Height_Filter', *Height_FilterValue*, ...)` specifies the minimum height for reported peaks. Peaks with heights below this value are not included in the output list *Peaks*. *Height_FilterValue* must be a positive real value. Default is 0.

Peaks = mspeaks(*MZ*, *Intensities*, ...'ShowPlot', *ShowPlotValue*, ...) controls the display of a plot of the original and the smoothed signal, with the peaks included in the output matrix *Peaks* marked. Choices are true, false, or *I*, an integer specifying the index of a spectrum in *Intensities*. If set to true, the first spectrum in *Intensities* is plotted. Default is:

- false — When return values are specified.
- true — When return values are not specified.

Examples

1. Load a MAT file, included with Bioinformatics Toolbox, which contains mass spectrometry data variables, including MZ_lo_res, a vector of m/z values for a set of spectra, and Y_lo_res, a matrix of intensity values for a set of mass spectra that share the same m/z range.

```
load sample_lo_res
```

2. Adjust the baseline of the eight spectra stored in Y_lo_res.

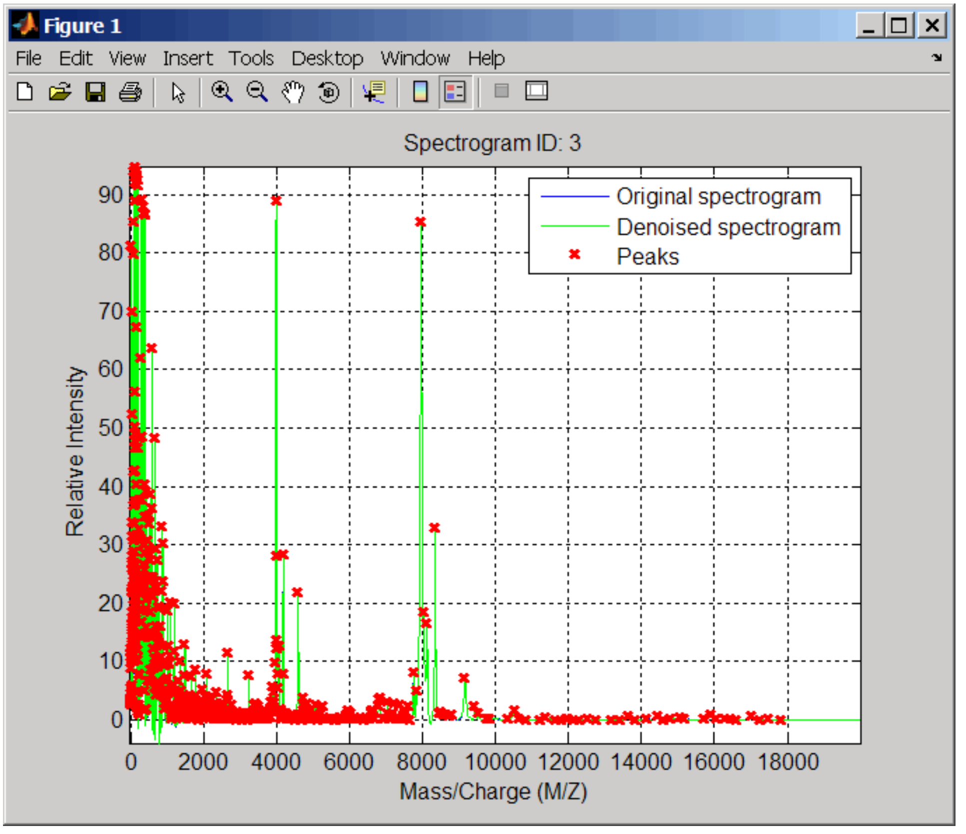
```
YB = msbackadj(MZ_lo_res,Y_lo_res);
```

3. Convert the raw mass spectrometry data to a peak list by finding the relevant peaks in each spectrum.

```
P = mspeaks(MZ_lo_res,YB);
```

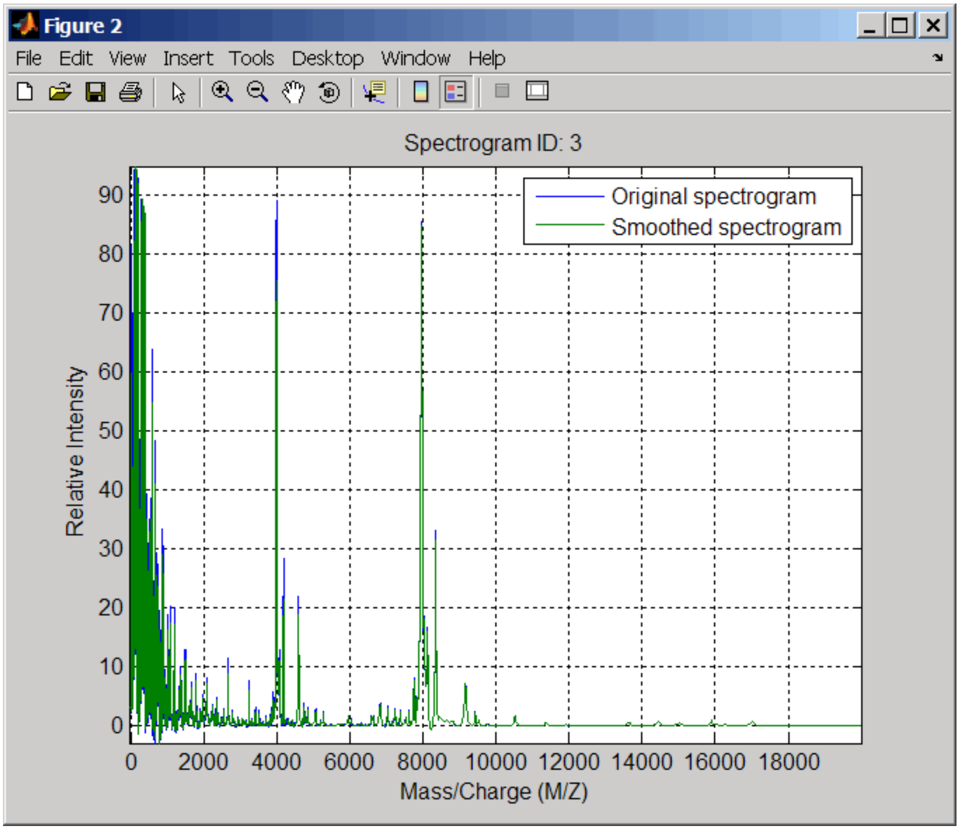
4. Plot the third spectrum in YB, the matrix of baseline-corrected intensity values, with the detected peaks marked.

```
P = mspeaks(MZ_lo_res,YB,'SHOWPLOT',3);
```

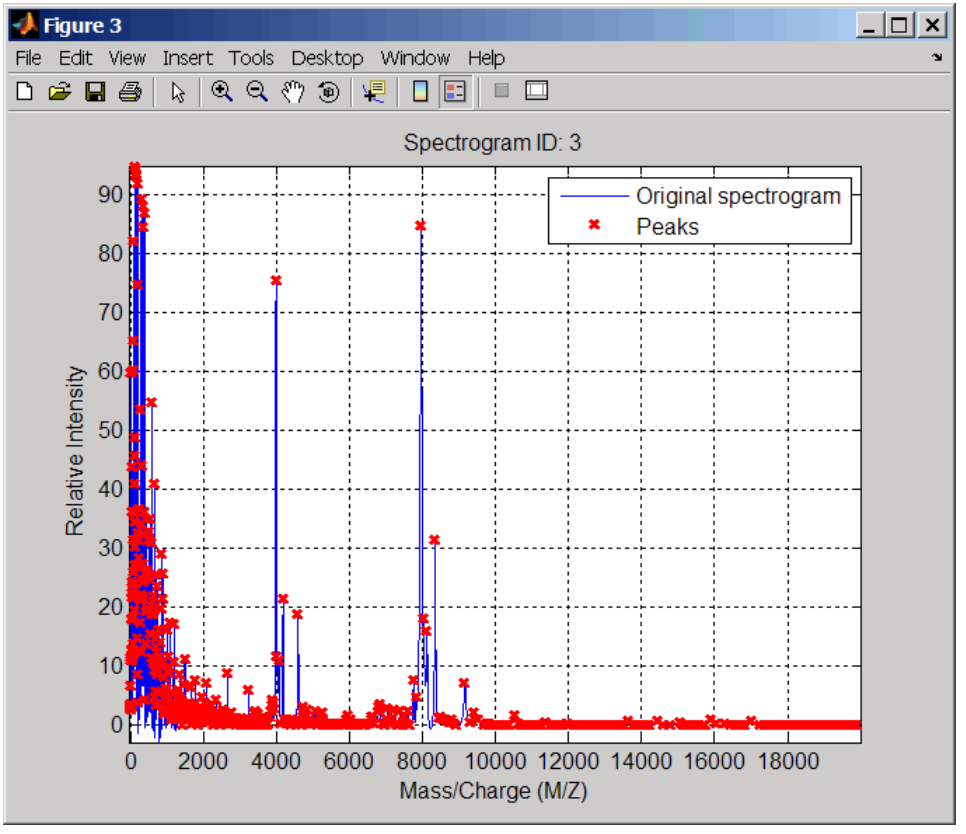


5 Smooth the signal using the `mslowess` function. Then convert the smoothed data to a peak list by finding relevant peaks and plot the third spectrum.

```
YS = mslowess(MZ_lo_res,YB,'SHOWPLOT',3);
```

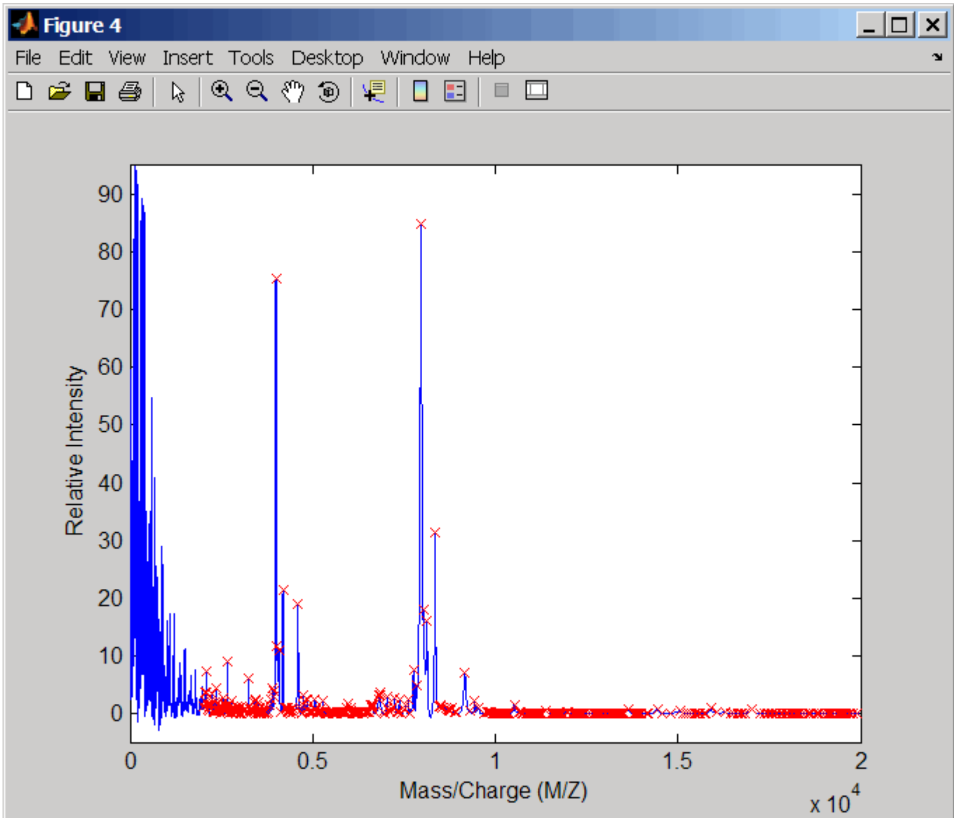



```
P = mspeaks(MZ_lo_res,YS,'DENOISING',false,'SHOWPLOT',3);
```



6 Use the `cellfun` function to remove all peaks with m/z values less than 2000 from the eight peaks lists in output `P`. Then plot the peaks of the third spectrum (in red) over its smoothed signal (in blue).

```
Q = cellfun(@(p) p(p(:,1)>2000,:),P,'UniformOutput',false);
figure
plot(MZ_lo_res,YS(:,3),'b',Q{3}(:,1),Q{3}(:,2),'rx')
xlabel('Mass/Charge (M/Z)')
ylabel('Relative Intensity')
axis([0 20000 -5 95])
```



References

[1] Morris, J.S., Coombes, K.R., Koomen, J., Baggerly, K.A., and Kobayash, R. (2005) Feature extraction and quantification for mass spectrometry in biomedical applications using the mean spectrum. Bioinfomatics *21:9*, 1764–1775.

[2] Yasui, Y., Pepe, M., Thompson, M.L., Adam, B.L., Wright, G.L., Qu, Y., Potter, J.D., Winget, M., Thornquist, M., and Feng, Z. (2003) A data-analytic strategy for protein biomarker discovery: profiling of

high-dimensional proteomic data for cancer detection. Biostatistics *4:3*, 449–463.

[3] Donoho, D.L., and Johnstone, I.M. (1995) Adapting to unknown smoothness via wavelet shrinkage. J. Am. Statist. Asso. *90*, 1200–1224.

[4] Strang, G., and Nguyen, T. (1996) Wavelets and Filter Banks (Wellesley: Cambridge Press).

[5] Coombes, K.R., Tsavachidis, S., Morris, J.S., Baggerly, K.A., Hung, M.C., and Kuerer, H.M. (2005) Improved peak detection and quantification of mass spectrometry data acquired from surface-enhanced laser desorption and ionization by denoising spectra with the undecimated discrete wavelet transform. Proteomics *5(16)*, 4107–4117.

See Also

Bioinformatics Toolbox functions: `msbackadj`, `msdotplot`, `mslowess`, `mspalign`, `msppresample`, `mssgolay`

msppresample

Purpose

Resample mass spectrometry signal while preserving peaks

Syntax

```
[MZ, Intensities] = msppresample(Peaks, N)
[MZ, Intensities] = msppresample(Peaks, N,
...'Range', RangeValue, ...)
[MZ, Intensities] = msppresample(Peaks, N, ...'FWHH',
    FWHHValue, ...)
[MZ, Intensities] = msppresample(Peaks, N, ...'ShowPlot',
    ShowPlotValue, ...)
```

Arguments

Peaks — Either of the following:

- Two-column matrix, where the first column contains mass/charge (m/z) values and the second column contains ion intensity values.
- Cell array of peak lists, where each element is a two-column matrix of m/z values and ion intensity values, and each element corresponds to a spectrum or retention time.

Note You can use the `mzxml2peaks` function or the `mspeaks` function to create the *Peaks* matrix or cell array.

N — Integer specifying the number of equally spaced points (m/z values) in the resampled signal.

RangeValue — 1-by-2 vector specifying the minimum and maximum m/z values for the output matrix *Intensities*. *RangeValue* must be within `[min(`*inputMZ*`) max(`*inputMZ*`)]`, where *inputMZ* is the concatenated m/z values from the input *Peaks*. Default is the full range `[min(`*inputMZ*`) max(`*inputMZ*`)]`.

FWHHValue	Value that specifies the full width at half height (FWHH) in m/z units. The FWHH is used to convert each peak to a Gaussian shaped curve. Default is `median(diff(`*`inputMZ`*`))/2`, where *`inputMZ`* is the concatenated m/z values from the input *`Peaks`*. The default is a rough approximation of resolution observed in the input data, *`Peaks`*.

Tip To ensure that the resolution of the peaks is preserved, set *`FWHHValue`* to half the distance between the two peaks of interest that are closest to each other.

ShowPlotValue	Controls the display of a plot of an original and resampled spectrum. Choices are `true`, `false`, or *`I`*, an integer specifying the index of a spectrum in *`Intensities`*. If set to `true`, the first spectrum in *`Intensities`* is plotted. Default is: • `false` — When return values are specified. • `true` — When return values are not specified.

Return Values

MZ	Vector of equally spaced, common mass/charge (m/z) values for a set of spectra. The number of elements in the vector equals *`N`* or the number of rows in matrix *`Intensities`*.
Intensities	Matrix of reconstructed intensity values for a set of mass spectra that share the same mass/charge (m/z) range. Each row corresponds to an m/z value, and each column corresponds to a spectrum or retention time. The number of rows equals *`N`* or the number of elements in vector *`MZ`*.

Description

[*MZ*, *Intensities*] = msppresample(*Peaks*, *N*) resamples *Peaks*, a mass spectrometry peak list, by converting centroided peaks to a semicontinuous, raw signal that preserves peak information. The resampled signal has *N* equally spaced points. Output *MZ* is a vector of *N* elements specifying the equally spaced, common m/z values for the spectra. Output *Intensities* is a matrix of reconstructed intensity values for a set of mass spectra that share the same m/z range. Each row corresponds to an m/z value, and each column corresponds to a spectrum or retention time. The number of rows equals *N*.

msppresample uses a Gaussian kernel to reconstruct the signal. The ion intensity at any given m/z value is taken from the maximum intensity of any contributing (overlapping) peaks.

Tip msppresample is useful to prepare a set of spectra for imaging functions such as msheatmap and preprocessing functions such as msbackadj and msnorm.

[*MZ*, *Intensities*] = msppresample(*Peaks*, *N*, ... '*PropertyName*', *PropertyValue*, ...) calls msppresample with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

[*MZ*, *Intensities*] = msppresample(*Peaks*, *N*, ...'Range', *RangeValue*, ...) specifies an m/z range for the output matrix *Intensities* using the minimum and maximum m/z values specified in the 1-by-2 vector *RangeValue*. *RangeValue* must be within [min(*inputMZ*) max(*inputMZ*)], where *inputMZ* is the concatenated m/z values from the input *Peaks*. Default is the full range [min(*inputMZ*) max(*inputMZ*)]

[*MZ*, *Intensities*] = msppresample(*Peaks*, *N*, ...'FWHH', *FWHHValue*, ...) sets the full width at half height (FWHH) in m/z units. The FWHH is used to convert each peak to a Gaussian shaped curve. Default is `median(diff(inputMZ))/2`, where *`inputMZ`* is the concatenated m/z values from the input *`Peaks`*. The default is a rough approximation of resolution observed in the input data, *`Peaks`*.

Tip To ensure that the resolution of the peaks is preserved, set *`FWHHValue`* to half the distance between the two peaks of interest that are closest to each other.

`[MZ, Intensities] = msppresample(Peaks, N, ...'ShowPlot', ShowPlotValue, ...)` controls the display of a plot of an original and resampled spectrum. Choices are `true`, `false`, or *`I`*, an integer specifying the index of a spectrum in *`Intensities`*. If set to `true`, the first spectrum in *`Intensities`* is plotted. Default is:

- `false` — When return values are specified.
- `true` — When return values are not specified.

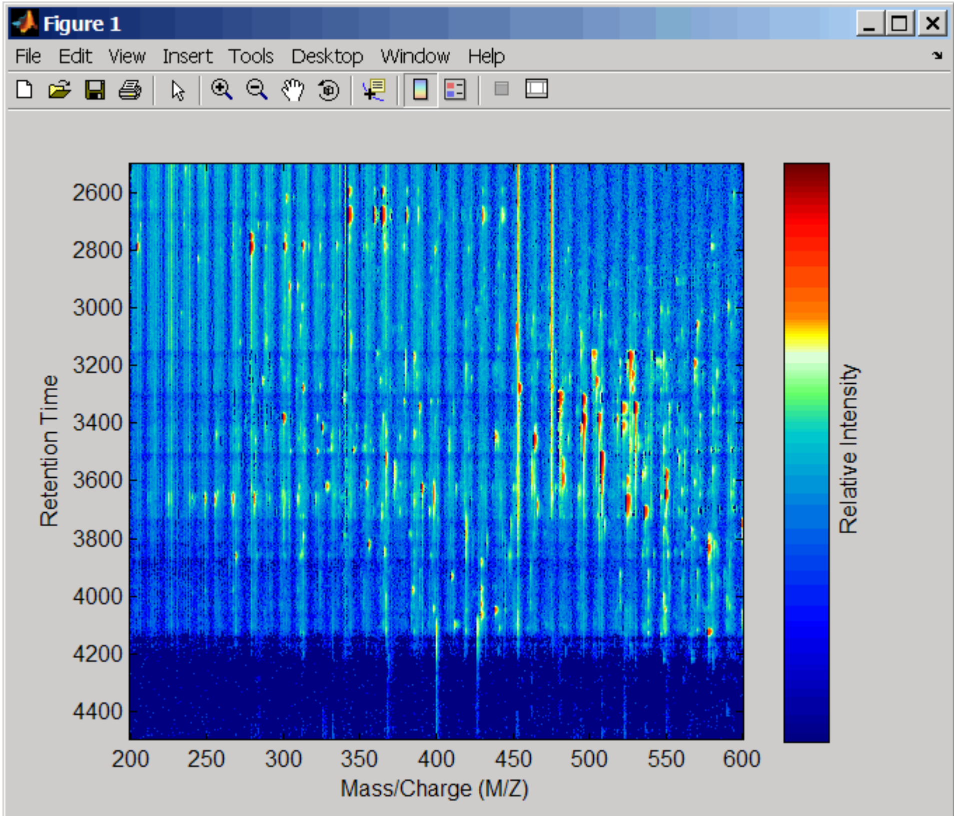
Examples

1 Load a MAT file, included with Bioinformatics Toolbox, which contains liquid chromatography/mass spectrometry (LC/MS) data variables, including `peaks`, a cell array of peak lists, where each element is a two-column matrix of m/z values and ion intensity values, and each element corresponds to a spectrum or retention time.

```
load lcmsdata
```

2 Resample the data, specifying 5000 m/z values in the resampled signal. Then create a heat map of the LC/MS data.

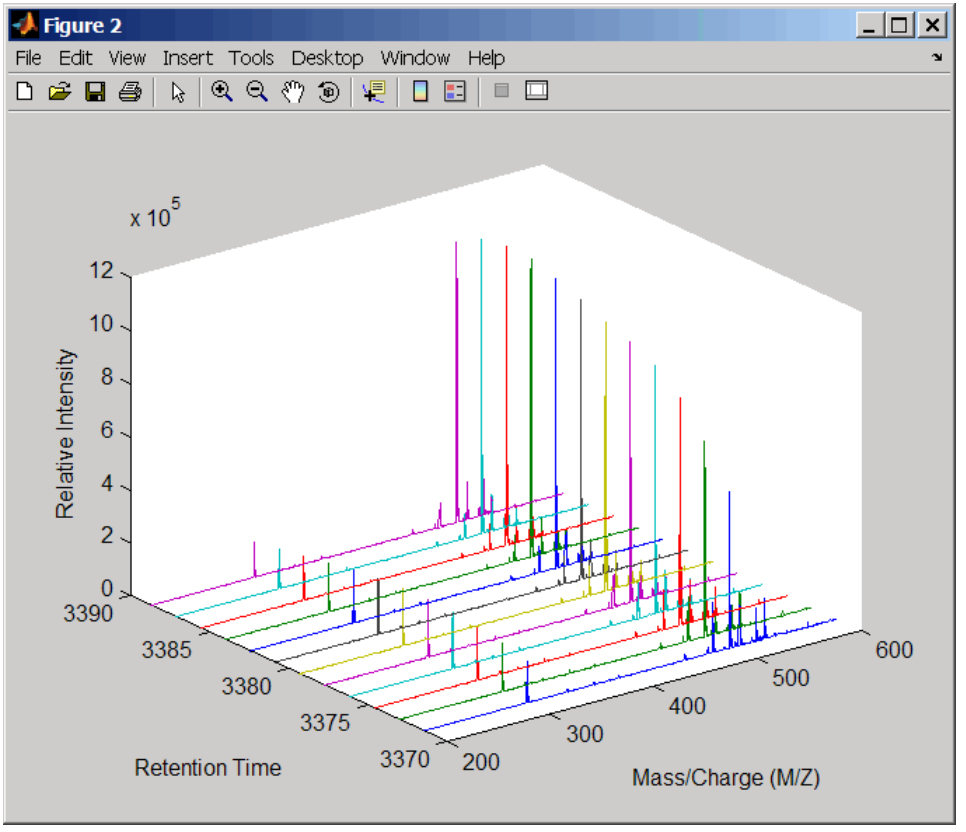
```
[MZ,Y] = msppresample(peaks,5000);
msheatmap(MZ,ret_time,log(Y))
```



3 Plot the reconstructed profile spectra between two retention times.

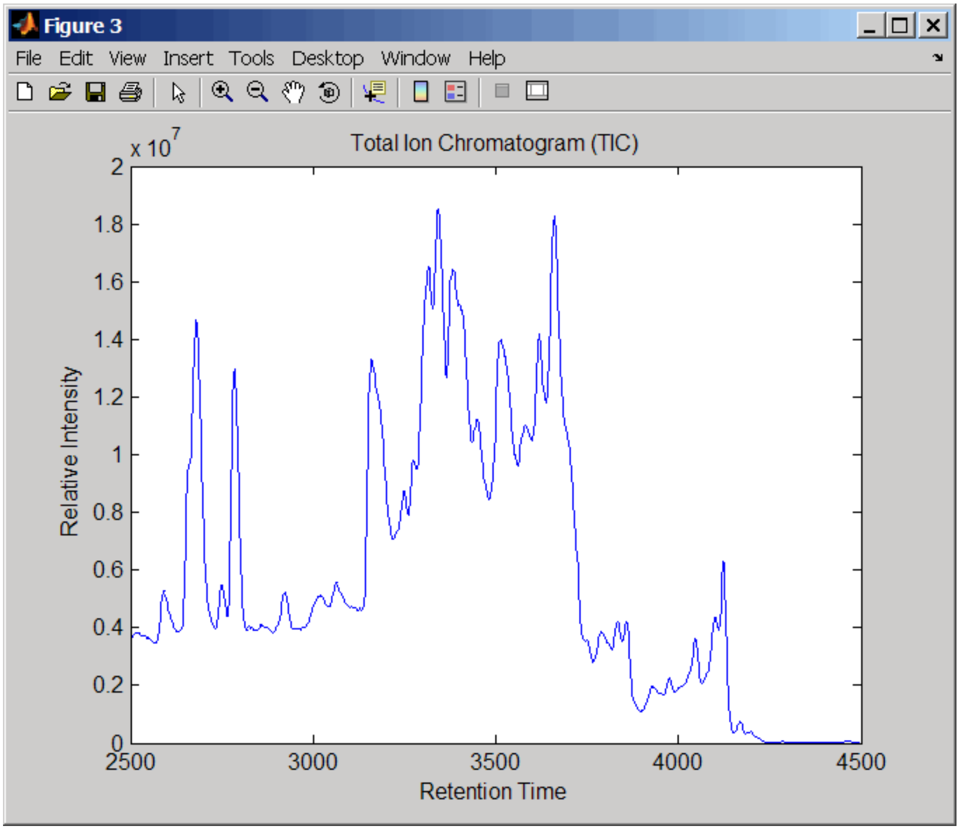
```
figure
t1 = 3370;
t2 = 3390;
h = find(ret_time>t1 & ret_time<t2);
[MZ,Y] = msppresample(peaks(h),10000);
plot3(repmat(MZ,1,numel(h)),repmat(ret_time(h)',10000,1),Y)
xlabel('Mass/Charge (M/Z)')
ylabel('Retention Time')
```

```
zlabel('Relative Intensity')
```



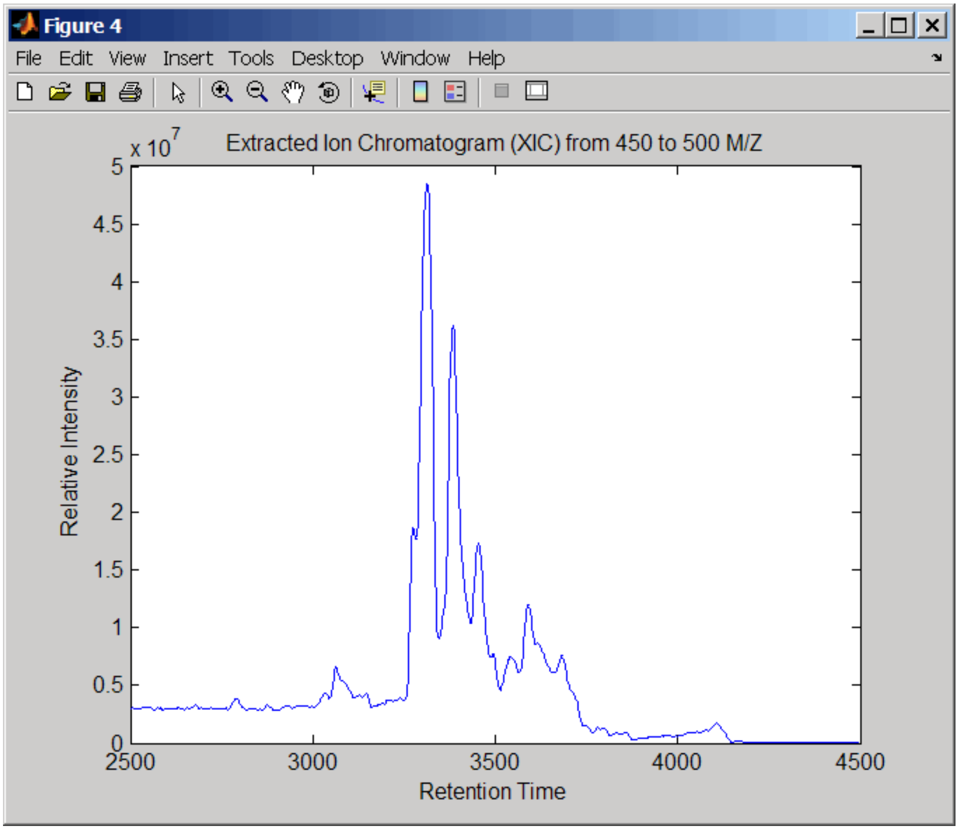
4 Resample the data to plot the Total Ion Chromatogram (TIC).

```
figure
[MZ,Y] = msppresample(peaks,5000);
plot(ret_time,sum(Y))
title('Total Ion Chromatogram (TIC)')
xlabel('Retention Time')
ylabel('Relative Intensity')
```



5 Resample the data to plot the Extracted Ion Chromatogram (XIC) in the 450 to 500 m/z range.

```
figure
[MZ,Y] = msppresample(peaks,5000,'Range',[450 500]);
plot(ret_time,sum(Y))
title('Extracted Ion Chromatogram (XIC) from 450 to 500 M/Z')
xlabel('Retention Time')
ylabel('Relative Intensity')
```



See Also

Bioinformatics Toolbox functions: `msdotplot`, `mspeaks`, `mspalign`, `msresample`, `mzxml2peaks`, `mzxmlread`

msresample

Purpose

Resample mass spectrometry signal

Syntax

```
[MZout, Yout] = msresample(MZ, Y, N)
msresample(..., 'PropertyName', PropertyValue,...)
msresample(..., 'Uniform', UniformValue)
msresample(..., 'Range', RangeValue)
msresample(..., 'Missing', MissingValue)
msresample(..., 'Window', WindowValue)
msresample(..., 'Cutoff', CutoffValue)
msresample(..., 'ShowPlot', ShowPlotValue)
```

Arguments

MZ	Mass/charge vector with the range of ions in the spectra.
Y	Ion intensity vector with the same length as the mass/charge vector (*MZ*). *Y* can also be a matrix with several spectra that share the same mass/charge (*MZ*) range.
N	Total number of samples.

Description

`[MZout, Yout] = msresample(MZ, Y, N)` resamples a raw mass spectrum (*Y*). The output spectrum will have *N* samples with a spacing that increases linearly within the range `[min(MZ) max(MZ)]`. *MZ* can be a linear or a quadratic function of its index. When input arguments are set such that down-sampling takes place, `msresample` applies a lowpass filter before resampling to minimize aliasing.

For the antialias filter, `msresample` uses a linear-phase FIR filter with a least-squares error minimization. The cu-off frequency is set by the largest down-sampling ratio when comparing the same regions in the *MZ* and *MZout* vectors.

Note `msresample` is particularly useful when you have spectra with different mass/charge vectors and you want to match the scales.

---

msresample(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

msresample(..., 'Uniform', *UniformValue*), when *UniformValue* is true, forces the vector *MZ* to be uniformly spaced. The default value is false.

msresample(..., 'Range', *RangeValue*) specifies a 1-by-2 vector with the mass/charge range for the output spectrum (Yout). *RangeValue* must be within [min(*MZ*) max(*MZ*)]. The default value is the full range [min(*MZ*) max(*MZ*)].

msresample(..., 'Missing', *MissingValue*), when *MissingValue* is true, analyzes the mass/charge vector (*MZ*) for dropped samples. The default value is false. If the down-sample factor is large, checking for dropped samples might not be worth the extra computing time. Dropped samples can only be recovered if the original MZ values follow a linear or a quadratic function of the *MZ* vector index.

msresample(..., 'Window', *WindowValue*) specifies the window used when calculating parameters for the lowpass filter. Enter 'Flattop', 'Blackman', 'Hamming', or 'Hanning'. The default value is 'Flattop'.

msresample(..., 'Cutoff', *CutoffValue*) specifies the cutoff frequency. Enter a scalar value between 0 and 1 (Nyquist frequency or half the sampling frequency). By default, msresample estimates the cutoff value by inspecting the mass/charge vectors (*MZ*, MZout). However, the cutoff frequency might be underestimated if *MZ* has anomalies.

msresample(..., 'ShowPlot', *ShowPlotValue*) plots the original and the resampled spectrum. When msresample is called without output arguments, the spectra are plotted unless *ShowPlotValue* is false. When *ShowPlotValue* is true, only the first spectrum in Y is plotted. *ShowPlotValue* can also contain an index to one of the spectra in Y.

Examples

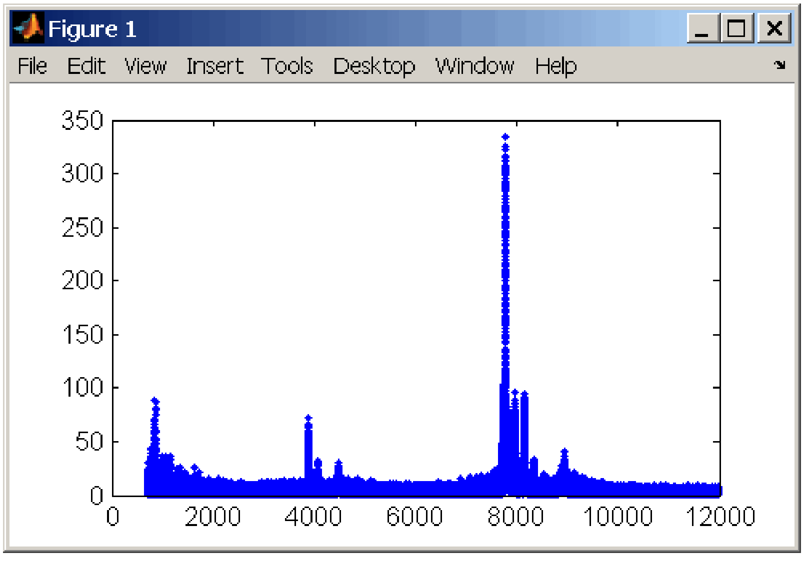
1. Load mass spectrometry data and extract m/z and intensity value vectors

```
load sample_hi_res;
mz = MZ_hi_res;
y = Y_hi_res;
```

2 Plot original data to a lower resolution.

```
plot(mz, y, '.')
```

MATLAB draws a figure.



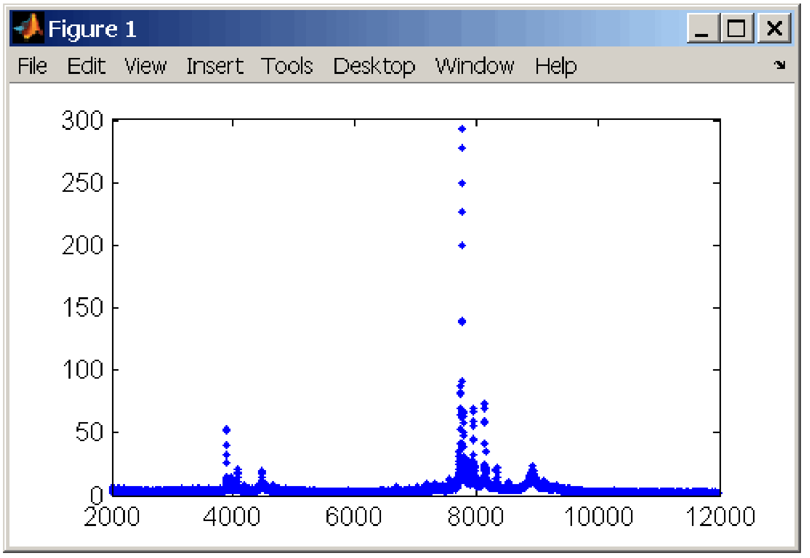
3 Resample data

```
[mz1,y1] = msresample(mz, y, 10000, 'range',[2000 max(mz)]);
```

4 Plot resampled data

```
plot(mz1,y1,'.')
```

MATLAB draws a figure with the down sampled data.



See Also

Bioinformatics Toolbox functions: `msalign`, `msbackadj`, `msheatmap`, `mslowess`, `msnorm`, `msppresample`, `mssgolay`, `msviewer`

mssgolay

Purpose

Smooth mass spectrum with least-squares polynomial

Syntax

```
Yout = mssgolay(MZ, Y)
mssgolay(..., 'PropertyName', PropertyValue,...)
mssgolay(..., 'Span', SpanValue)
mssgolay(..., 'Degree', DegreeValue)
mssgolay(..., 'ShowPlot', ShowPlotValue)
```

Arguments

MZ	Mass/charge vector with the range of ions in the spectra.
Y	Ion intensity vector with the same length as the mass/charge vector (*MZ*). *Y* can also be a matrix with several spectra that share the same mass/charge (*MZ*) range.

Description

`Yout = mssgolay(MZ, Y)` smoothes a raw mass spectrum (*Y*) using a least squares digital polynomial filter (Savitzky and Golay filters). The default span or frame is `15` samples.

`mssgolay(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`mssgolay(..., 'Span', SpanValue)` modifies the frame size for the smoothing function. If *SpanValue* is greater than `1`, the window is the size of *SpanValue* in samples independent of the *MZ* vector. Higher values will smooth the signal more with an increase in computation time. If *SpanValue* is less than `1`, the window size is a fraction of the number of points in the data (*MZ*). For example, if *SpanValue* is `0.05`, the window size is equal to `5%` of the number of points in *MZ*.

Note 1) The original algorithm by Savitzky and Golay assumes a uniformly spaced mass/charge vector (*MZ*), while mssgolay also allows one that is not uniformly spaced. Therefore, the sliding frame for smoothing is centered using the closest samples in terms of the *MZ* value and not in terms of the *MZ* index.

2) When the vector *MZ* does not have repeated values or NaNs, the algorithm is approximately twice as fast.

3) When the vector *MZ* is evenly spaced, the least-squares fitting is performed once so that the spectrum is filtered with the same coefficients, and the speed of the algorithm increases considerably.

4) If the vector *MZ* is evenly spaced and *SpanValue* is even, Span is incriminated by 1 to include both edge samples in the frame.

---

mssgolay(..., 'Degree', *DegreeValue*) specifies the degree of the polynomial (*DegreeValue*) fitted to the points in the moving frame. The default value is 2. *DegreeValue* must be smaller than *SpanValue*.

mssgolay(..., 'ShowPlot', *ShowPlotValue*) plots smoothed spectra over the original. When mssgolay is called without output arguments, the spectra are plotted unless *ShowPlotValue* is false. When *ShowPlotValue* is true, only the first spectrum in *Y* is plotted. *ShowPlotValue* can also contain an index to one of the spectra in *Y*.

Examples

```
load sample_lo_res
YS = mssgolay(MZ_low_res, Y_low_res(:,1));
plot(MZ,[Y(:,1) YS])
```

See Also

Bioinformatics Toolbox functions msalign, msbackadj, msheatmap, mslowess, msnorm, mspeaks, msresample, msviewer

Purpose

Explore mass spectrum or set of mass spectra

Syntax

```
msviewer(MZ, Y)
msviewer(..., 'Markers', MarkersValue)
msviewer(..., 'Group', GroupValue)
```

Arguments

`MZ`	Mass/charge vector with the range of ions in the spectra.
`Y`	Ion intensity vector with the same length as the mass/charge vector (`MZ`). `Y` can also be a matrix with several spectra that share the same mass/charge (`MZ`) range.

Description

`msviewer(MZ, Y)` creates a GUI to display and explore a mass spectrum (`Y`).

`msviewer(..., 'Markers', *MarkersValue*)`specifies a list of marker positions from the mass/charge vector (`MZ`) for exploration and easy navigation. Enter a column vector with `MZ` values.

`msviewer(..., 'Group', *GroupValue*)` specifies a class label for every spectrum with a different color for every class. Enter a column vector of size `[numSpectra x 1]` with integers. The default value is `[numSpectra]`.

MSViewer GUI features include the following:

- Plot mass spectra. The spectra are plotted with different colors according to their class labels.
- An overview displays a full spectrum, and a box indicates the region that is currently displayed in the main window.
- Five different zoom in options, one zoom out option, and a reset view option resize the spectrum.
- Add/focus/move/delete marker operations

- Import/Export markers from/to MATLAB workspace
- Print and preview the spectra plot
- Print the spectra plot to a MATLAB figure window

MSViewer has five components:

- Menu bar: **File**, **Tools**, **Window**, and **Help**
- Toolbar: Zoom XY, Zoom X, Zoom Y, Reset view, Zoom out, and Help
- Main window: display the spectra
- Overview window: display the overview of a full spectrum (the average of all spectra in display)
- Marker control panel: a list of markers, Add marker, Delete marker, up and down buttons

Examples

1. Load and plot sample data

```
load sample_lo_res
msviewer(MZ_lo_res, Y_lo_res)
```

2. Add a marker by pointing to a mass peak, right-clicking, and then clicking **Add Marker**.

3. From the **File** menu, select

   - **Import Markers from Workspace** — Opens the Import Markers From MATLAB Workspace dialog. The dialog should display a list of double `Mx1` or `1xM` variables. If the selected variable is out of range, the viewer displays an error message
   - **Export Markers to Workspace** — Opens the Export Markers to MATLAB Workspace dialog. You can enter a variable name for the markers. All markers are saved. If there is no marker available, this menu item should be disabled.

- **Print to Figure** — Prints the spectra plot in the main display to a MATLAB figure window

4 From the **Tools** menu, click

- **Add Marker** — Opens the Add Marker dialog. Enter an m/z marker.
- **Delete Marker** — Removes the currently selected m/z marker from the **Markers** (m/z) list.
- **Next Marker** or **Previous Marker** — Moves the selection up and down the **Markers** (m/z) list.
- **Zoom XY**, **Zoom X**, **Zoom Y**, or **Zoom Out** — Changes the cursor from an arrow to crosshairs. Left-click and drag a rectangle box over an area and then release the mouse button. The display zooms the area covered by the box.

5 Move the cursor to the range window at the bottom. Click and drag the view box to a new location.

See Also

Bioinformatics Toolbox functions `msalign`, `msbackadj`, `mslowess`, `msnorm`, `msheatmap`, `msresample`, `mssgolay`

Purpose Align multiple sequences using progressive method

Syntax

```
SeqsMultiAligned = multialign(Seqs)
SeqsMultiAligned = multialign(Seqs, Tree)
multialign(..., 'PropertyName', PropertyValue,...)
multialign(..., 'Weights', WeightsValue)
multialign(..., 'ScoringMatrix', ScoringMatrixValue)
multialign(..., 'SMInterp', SMInterpValue)
multialign(..., 'GapOpen', GapOpenValue)
multialign(..., 'ExtendGap', ExtendGapValue)
multialign(..., 'DelayCutoff', DelayCutoffValue)
multialign(..., 'JobManager', JobManagerValue)
multialign(..., 'WaitInQueue', WaitInQueueValue)
multialign(..., 'Verbose', VerboseValue)
multialign(..., 'ExistingGapAdjust',
ExistingGapAdjustValue)
multialign(..., 'TerminalGapAdjust',
TerminalGapAdjustValue)
```

Arguments

Seqs	Vector of structures with the fields 'Sequence' for the residues and 'Header' or 'Name' for the labels. *Seqs* may also be a cell array of strings or a char array.
SeqsMultiAligned	Vector of structures (same as *Seqs*) but with the field 'Sequence' updated with the alignment. When *Seqs* is a cell or char array, *SeqsMultiAligned* is a char array with the output alignment following the same order as the input.

Tree	Phylogenetic tree calculated with either of the functions `seqlinkage` or `seqneighjoin`.
WeightsValue	Property to select the sequence weighting method. Enter either `'THG'` (default) or `'equal'`.
ScoringMatrixValue	Property to select or specify the scoring matrix. Enter an `[MxM]` matrix or `[MxMxN]` array of matrixes with`N` user-defined scoring matrices. *ScoringMatrixValue*may also be a cell array of strings with matrix names.The default is the `BLOSUM80` to `BLOSUM30` series for amino acids or a fixed matrix NUC44 for nucleotides. When passing your own series of scoring matrices make sure all of them share the same scale.
SMInterpValue	Property to specify whether linear interpolation of the scoring matrices is on or off. When `false`, scoring matrix is assigned to a fixed range depending on the distances between the two profiles (or sequences) being aligned. Default is `true`.
GapOpenValue	Scalar or a function specified using `@`. If you enter a function,`multialign` passes four values to the function: the average score for two matched residues (`sm`), the average score for two mismatched residues (`sx`), and, the length of both profiles or sequences (`len1`, `len2`). Default is `@(sm,sx,len1,len2) 5*sm`.

ExtendGapValue	Scalar or a function specified using `@`. IF you enter a function, `multiialign` passes four values to the function: the average score for two matched residues (`sm`), the average score for two mismatched residues (`sx`), and the length of both profiles or sequences (`len1`, `len2`). Default is `@(sm,sx,len1,len2) sm/4`.
DelayCutoffValue	Property to specify the threshold delay of divergent sequences. The default is unity where sequences with the closest sequence farther than the median distance are delayed.
JobManagerValue	JobManager object representing an available distributed MATLAB resource. Enter a jobmanager object returned by the Distributed Computing Toolbox function `findResource`.
WaitInQueueValue	Property to control waiting for a distributed MATLAB resource to be available. Enter either `true` or `false`. The default value is `false`.
VerboseValue	Property to control displaying the sequences with sequence information. Default value is `false`.
ExistingGagAdjustValue	Property to control automatic adjustment based on existing gaps. Default value is `true`.
TerminalGapAdjustValue	Property to adjusts the penalty for opening a gap at the ends of the sequence. Default value is `false`.

Description

SeqsMultiAligned = multialign(*Seqs*) performs a progressive multiple alignment for a set of sequences (*Seqs*). Pair-wise distances between sequences are computed after pair-wise alignment with the Gonnet scoring matrix and then by counting the proportion of sites at which each pair of sequences are different (ignoring gaps). The guide tree is calculated by the neighbor-joining method assuming equal variance and independence of evolutionary distance estimates.

SeqsMultiAligned = multialign(*Seqs*, *Tree*) uses a tree (*Tree*) as a guide for the progressive alignment. The sequences (*Seqs)* should have the same order as the leaves in the tree (*Tree*) or use a field ('Header' or 'Name') to identify the sequences.

multialign(..., '*PropertyName*', *PropertyValue,...*) enters optional arguments as property name/value pairs.

multialign(..., 'Weights', *WeightsValue*) selects the sequence weighting method. Weights emphasize highly divergent sequences by scaling the scoring matrix and gap penalties. Closer sequences receive smaller weights.

Values of the property Weights:

- 'THG'(default) — Thompson-Higgins-Gibson method using the phylogenetic tree branch distances weighted by their thickness.
- 'equal' — Assigns same weight to every sequence.

multialign(..., 'ScoringMatrix', *ScoringMatrixValue*) selects the scoring matrix (*ScoringMatrixValue*) for the progressive alignment. Match and mismatch scores are interpolated from the series of scoring matrices by considering the distances between the two profiles or sequences being aligned. The first matrix corresponds to the smallest distance and the last matrix to the largest distance. Intermediate distances are calculated using linear interpolation.

multialign(..., 'SMInterp', *SMInterpValue*), when *SMInterpValue* is false, turns off the linear interpolation of the scoring matrices. Instead, each supplied scoring matrix is assigned to a fixed range depending on the distances between the two profiles or sequences being aligned.

`multialign(..., 'GapOpen', GapOpenValue)` specifies the initial penalty for opening a gap.

`multialign(..., 'ExtendGap', ExtendGapValue)` specifies the initial penalty for extending a gap.

`multialign(..., 'DelayCutoff', DelayCutoffValue)` specifies a threshold to delay the alignment of divergent sequences whose closest neighbor is farther than

```
(DelayCutoffValue) * (median patristic distance
between sequences)
```

`multialign(..., 'JobManager', JobManagerValue)` distributes pair-wise alignments into a cluster of computers using Distributed Computing Toolbox.

`multialign(..., 'WaitInQueue', WaitInQueueValue)` when *`WaitInQueueValue`* is true, waits in the job manager queue for an available worker. When *`WaitInQueueValue`* is `false` (default) and there are no workers immediately available, `multialign` errors out. Use this property with Distributed Computing Toolbox and the `multialign` property `WaitInQueue`.

`multialign(..., 'Verbose', VerboseValue)`, when *`VerboseValue`* is `true`, turns on verbosity.

The remaining input optional arguments are analogous to the function `profalign` and are used through every step of the progressive alignment of profiles.

`multialign(..., 'ExistingGapAdjust', ExistingGapAdjustValue)`, if *`ExistingGapAdjustValue`* is `false`, turns off the automatic adjustment based on existing gaps of the position-specific penalties for opening a gap.

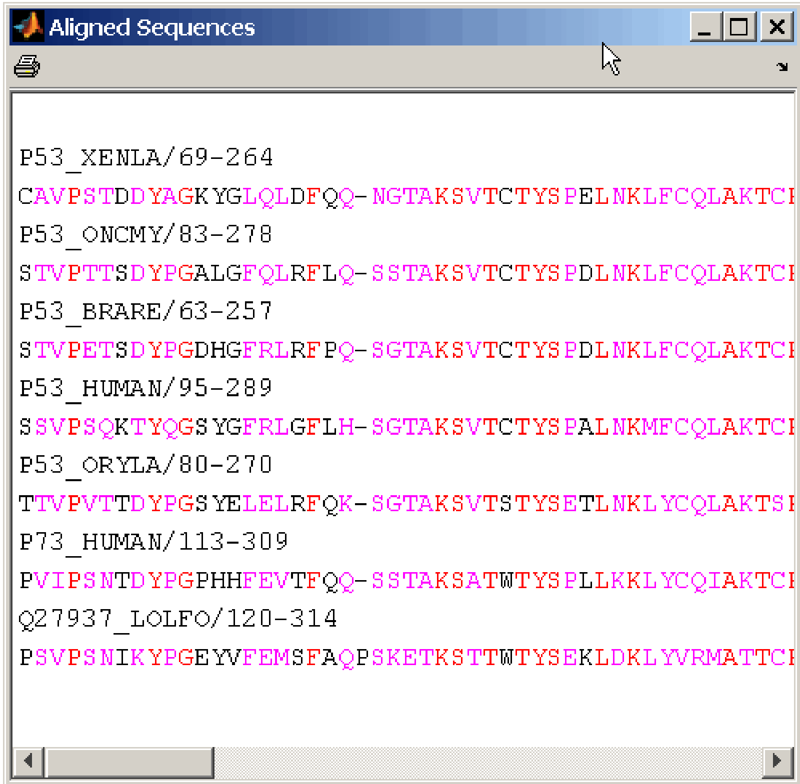
When *`ExistingGapAdjustValue`* is true, for every profile position, `profalign` proportionally lowers the penalty for opening a gap toward the penalty of extending a gap based on the proportion of gaps found in the contiguous symbols and on the weight of the input profile.

`multialign(..., 'TerminalGapAdjust', TerminalGapAdjustValue)`, when *`TerminalGapAdjustValue`* is `true`, adjusts the penalty for opening a gap at the ends of the sequence to be equal to the penalty for extending a gap.

Example 1

1. Align seven cellular tumor antigen p53 sequences.

```
p53 = fastaread('p53samples.txt')
ma = multialign(p53,'verbose',true)
showalignment(ma)
```

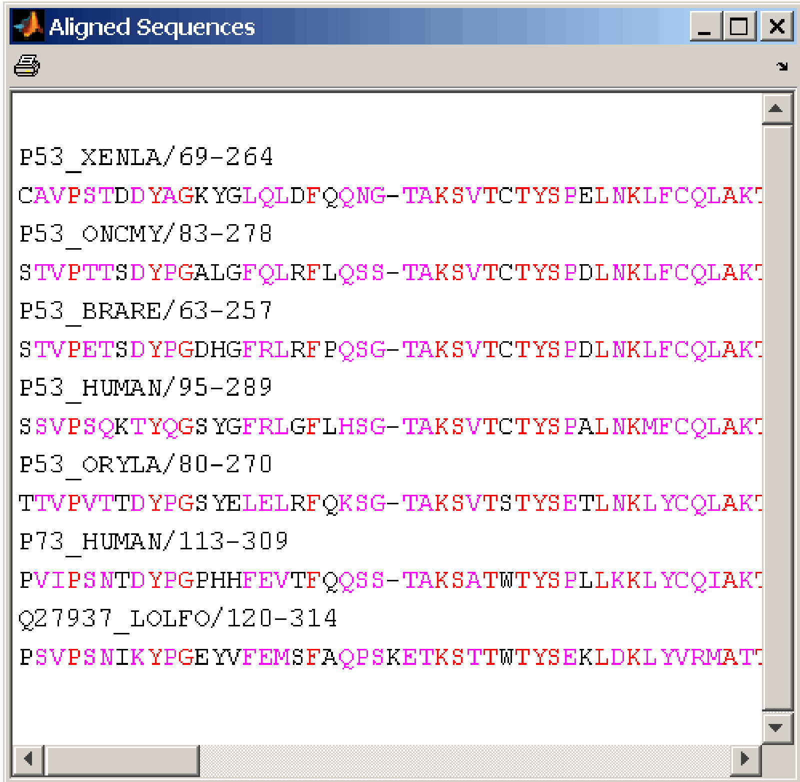


2 Use an UPGMA phylogenetic tree instead as a guiding tree.

```
dist = seqpdist(p53,'ScoringMatrix',gonnet);
tree = seqlinkage(dist,'UPGMA',p53)

Phylogenetic tree object with 7 leaves (6 branches)
```

3 Score the progressive alignment with the PAM family.

```
ma = multialign(p53,tree,'ScoringMatrix',...
                {'pam150','pam200','pam250'})
showalignment(ma)
```



Example 2

1 Enter an array of sequences.

```
seqs = {'CACGTAACATCTC','ACGACGTAACATCTTCT','AAACGTAACATCTCGC'};
```

2 Promote terminations with gaps in the alignment.

```
multialign(seqs,'terminalGapAdjust',true)

ans =
--CACGTAACATCTC--
ACGACGTAACATCTTCT
-AAACGTAACATCTCGC
```

3 Compare alignment without termination gap adjustment.

```
multialign(seqs)

ans =
CA--CGTAACATCT--C
ACGACGTAACATCTTCT
AA-ACGTAACATCTCGC
```

See Also

Bioinformatics Toolbox functions: `hmmprofalign`, `multialignread`, `nwalign`, `profalign`, `seqprofile`, `seqconsensus`, `seqneighjoin`, `showalignment`

multialignread

Purpose

Read multiple-sequence alignment file

Syntax

```
S = multialignread(File)
[Headers, Sequences] = multialignread(File)
multialignread(..., 'PropertyName', PropertyValue,...)
multialignread(..., 'IgnoreGaps', IgnoreGapsValue)
```

Arguments

File	Multiple sequence alignment file (ASCII text file). Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text of a multiple sequence alignment file. You can read common multiple alignment file types, such as ClustalW (`.aln`) and GCG (`.msf`).
IgnoreGapsValue	Property to control removing gap symbols.

Description

`S = multialignread(File)` reads a multiple sequence alignment file. The file contains multiple sequence lines that start with a sequence header followed by an optional number (not used by `multialignread`) and a section of the sequence. The multiple sequences are broken into blocks with the same number of blocks for every sequence. (For an example, type `open aagag.aln`.) The output *S* is a structure array where `S.Header` contains the header information and `S.Sequence` contains the amino acid or nucleotide sequences.

`[Headers, Sequences] = multialignread(File)` reads the file into separate variables `Headers` and `Sequences`.

`multialignread(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`multialignread(..., 'IgnoreGaps', IgnoreGapsValue)`, when *IgnoreGapsValue* is `true`, removes any gap symbol (`'-'` or `'.'`) from the sequences. Default is `false`.

Examples

Read a multiple sequence alignment of the gag polyprotein for several HIV strains.

```
gagaa = multialignread('aagag.aln')

gagaa =

1x16 struct array with fields:
    Header
    Sequence
```

See Also

Bioinformatics Toolbox functions: `fastaread`, `gethmmalignment`, `multialign`, `seqconsensus`, `seqdisp`, `seqprofile`

multialignviewer

Purpose

Open viewer for multiple sequence alignments

Syntax

```
multialignviewer(Alignment)
multialignviewer(..., 'PropertyName', PropertyValue,...)
multialignviewer(..., 'Alphabet', AlphabetValue)
```

Description

The `multialignviewer` is an interactive graphical user interface (GUI) for viewing multiple sequence alignments.

`multialignviewer(`*`Alignment`*`)` loads a group of previously multiple aligned sequences into the viewer. *`Alignment`* is a structure with a field `Sequence`, a character array, or a file name.

`multialignviewer(..., '`*`PropertyName`*`', `*`PropertyValue`*`,...)` defines optional properties using property name/value pairs.

`multialignviewer(..., 'Alphabet', `*`AlphabetValue`*`)` specifies the alphabet type for the sequences . *`AlphabetValue`* can be `'AA'` for amino acids or `'NT'` for nucleotides. The default value is `'AA'`. If *`AlphabetValue`* is not specified, `multialignviewer` guesses the alphabet type.

Examples

```
multialignviewer('aagag.aln')
```

See Also

Bioinformatics Toolbox functions: `fastaread`, `gethmmalignment`, `multialign`, `multialignread`, `seqtool`

Purpose

Convert mzXML structure to peak list

Syntax

```
[Peaks, Times] = mzxml2peaks(mzXMLStruct)
[Peaks, Times] = mzxml2peaks(mzXMLStruct,
'Levels', LevelsValue)
```

Arguments

mzXMLStruct — mzXML structure, such as one created by the `mzxmlread` function. *mzXMLStruct* includes the following fields:

- `scan`
- `offset`
- `mzXML`

LevelsValue — Positive integer or vector of integers that specifies the level(s) of spectra in *mzXMLStruct* to convert, assuming the spectra are from tandem MS data sets. Default is `1`, which converts only the first-level spectra, that is spectra containing precursor ions. Setting *LevelsValue* to `2` converts only the second-level spectra, which are the fragment spectra (created from a precursor ion).

Return Values

Peaks	Either of the following: • Two-column matrix, where the first column contains mass/charge (m/z) values and the second column contains ion intensity values. • Cell array of peak lists, where each element is a two-column matrix of m/z values and ion intensity values, and each element corresponds to a spectrum or retention time.
Times	Vector of retention times associated with a liquid chromatography/mass spectrometry (LC/MS) or gas chromatography/mass spectrometry (GC/MS) data set. The number of elements in *Times* equals the number of elements in *Peaks*.

Description

[*Peaks*, *Times*] = mzxml2peaks(*mzXMLStruct*) extracts peak information from *mzXMLStruct*, an mzXML structure, and creates *Peaks*, a cell array of matrices containing mass/charge (m/z) values and ion intensity values, and *Times*, a vector of retention times associated with a liquid chromatography/mass spectrometry (LC/MS) or gas chromatography/mass spectrometry (GC/MS) data set.

[*Peaks*, *Times*] = mzxml2peaks(*mzXMLStruct*, 'Levels', *LevelsValue*) specifies the level(s) of the spectra in *mzXMLStruct* to convert, assuming the spectra are from tandem MS data sets. Default is 1, which converts only the first-level spectra, that is spectra containing precursor ions. Setting *LevelsValue* to 2 converts only the second-level spectra, which are the fragment spectra (created from a precursor ion).

Examples

1 Use the mzxmlread function to read an mzXML file into MATLAB as structure. Then extract the peak information of only the first-level ions from the structure.

```
mzxml_struct = mzxmlread('results.mzxml');
[peaks,time] = mzxml2peaks(mzxml_struct);
```

Note The file `results.mzxml` is not provided. Sample mzXML files can be found at

```
http://sashimi.sourceforge.net/repository.html
```

---

2 Create a dotplot of the LC/MS data.

```
msdotplot(peaks,time)
```

See Also

Bioinformatics Toolbox functions: `msdotplot`, `mspalign`, `msppresample`, `mzxmlread`

mzxmlread

Purpose

Read mzXML file into MATLAB as structure

Syntax

mzXMLStruct = mzxmlread(*File*)

Arguments

File	String containing a file name, or a path and file name, of an mzXML file that conforms to the mzXML 2.1 specification.

Description

mzXMLStruct = mzxmlread(*File*) reads an mzXML file, *File*, and then creates a MATLAB structure, *mzXMLStruct*.

File can be a file name, or a path and file name, of an mzXML file. The file must conform to the mzXML 2.1 specification at:

http://sashimi.sourceforge.net/schema_revision/mzXML_2.1/Doc/mzXML_2.1_tutorial.pdf

mzXMLStruct includes the following fields:

- scan
- offset
- mzXML

Tip If you receive any errors related to memory or Java heap space, try increasing your Java heap space as described at:

http://www.mathworks.com/support/solutions/data/1-18I2C.html

Examples

```
out = mzxmlread('results.mzxml');
% view a scan
m = out.scan{1}.peaks.mz(1:2:end);
z = out.scan{1}.peaks.mz(2:2:end);
bar(m,z)
```

Note The file `results.mzxml` is not provided. Sample mzXML files can be found at:

```
http://sashimi.sourceforge.net/repository.html
```

See Also

Bioinformatics Toolbox functions: `jcampread`, `msdotplot`, `mslowess`, `msppresample`, `mssgolay`, `msviewer`, `mzxml2peaks`

nmercount

Purpose

Count number of n-mers in nucleotide or amino acid sequence

Syntax

```
nmercount(Seq, Length)
nmercount(Seq, Length, C)
```

Arguments

Seq	Nucleotide or amino acid sequence. Enter a character string or a structure with the field `Sequence`.
Length	Length of n-mer to count. Enter an integer.

Description

`nmercount(`*Seq*`,` *Length*`)` counts the number of n-mers or patterns of a specific length in a sequence.

`nmercount(`*Seq*`,` *Length*`,` *C*`)` returns only the n-nmers with cardinality at least *C*.

Examples

Count the number of n-mers in an amino acid sequence and display the first six rows in the cell array.

```
S = getgenpept('AAA59174','SequenceOnly',true)
nmers = nmercount(S,4);
nmers(1:6,:)

ans =
    'apes'    [2]
    'dfrd'    [2]
    'eslk'    [2]
    'frdl'    [2]
    'gnys'    [2]
    'lkel'    [2]
```

See Also

Bioinformatics Toolbox functions: `basecount`, `codoncount`, `dimercount`

Purpose

Convert nucleotide sequence to amino acid sequence

Syntax

```
SeqAA = nt2aa(SeqNT)
SeqAA = nt2aa(..., 'Frame', FrameValue, ...)
SeqAA = nt2aa(..., 'GeneticCode', GeneticCodeValue, ...)
SeqAA = nt2aa(..., 'AlternativeStartCodons',
    AlternativeStartCodonsValue, ...)
```

Arguments

SeqNT	Either of the following: • String specifying a nucleotide sequence • MATLAB structure containing the field `Sequence` Valid characters include: • `A` • `C` • `G` • `T` • `U` • hyphen (`-`) **Note** Hyphens are valid only if the codon to which it belongs represents a gap, that is, the codon contains all hyphens. Example: `ACT---TGA` **Tip** Do not use a sequence with hyphens if you specify `'all'` for *FrameValue*.
FrameValue	Property to specify a reading frame. Choices are `1`, `2`, `3`, or `'all'`. Default is `1`. If *FrameValue* is `'all'`, then *SeqAA* is a 3-by-1 cell array.

GeneticCodeValue	Property to specify a genetic code. Enter a Code Number or a string with a Code Name from the tableGenetic Code on page 2-515. If you use a Code Name, you can truncate it to the first two characters. Default is `1` or `Standard`.
AlternativeStartCodonsValue	Property to control the translation of alternative codons. Choices are `true` or `false`. Default is `true`.

Genetic Code

Code Number	Code Name
1	`Standard`
2	`Vertebrate Mitochondrial`
3	`Yeast Mitochondrial`
4	`Mold, Protozoan, Coelenterate Mitochondrial, and Mycoplasma/Spiroplasma`
5	`Invertebrate Mitochondrial`
6	`Ciliate, Dasycladacean, and Hexamita Nuclear`
9	`Echinoderm Mitochondrial`
10	`Euplotid Nuclear`
11	`Bacterial and Plant Plastid`
12	`Alternative Yeast Nuclear`
13	`Ascidian Mitochondrial`
14	`Flatworm Mitochondrial`
15	`Blepharisma Nuclear`

Code Number	Code Name
16	Chlorophycean Mitochondrial
21	Trematode Mitochondrial
22	Scenedesmus Obliquus Mitochondrial
23	Thraustochytrium Mitochondrial

Return Values

SeqAA	String specifying an amino acid sequence.

Description

SeqAA = nt2aa(*SeqNT*) converts a nucleotide sequence to an amino acid sequence using the standard genetic code.

SeqAA = nt2aa(*SeqNT*, ...'*PropertyName*', *PropertyValue*, ...) calls nt2aa with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

SeqAA = nt2aa(..., 'Frame', *FrameValue*, ...) converts a nucleotide sequence for a specific reading frame to an amino acid sequence. Choices are 1, 2, 3, or 'all'. Default is 1. If *FrameValue* is 'all', then output *SeqAA* is a 3-by-1 cell array.

SeqAA = nt2aa(..., 'GeneticCode', *GeneticCodeValue*, ...) converts a nucleotide sequence to an amino acid sequence using a specific genetic code.

SeqAA = nt2aa(..., 'AlternativeStartCodons', *AlternativeStartCodonsValue*, ...) controls the translation of alternative start codons. By default, *AlternativeStartCodonsValue* is set to true, and if the first codon of a sequence is a known alternative start codon, the codon is translated to methionine.

If this option is set to `false`, then an alternative start codon at the start of a sequence is translated to its corresponding amino acid in the genetic code that you specify, which might not necessarily be methionine. For example, in the human mitochondrial genetic code, AUA and AUU are known to be alternative start codons.

For more details of alternative start codons, see

```
www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=t#SG1
```

Examples

The following example converts the gene ND1 on the human mitochondria genome to an amino acid sequence.

```
mitochondria = getgenbank('NC_001807', 'SequenceOnly', true)
ND1gene = mitochondria (3308:4264)
protein1 = nt2aa(ND1gene,'GeneticCode', 2)
protein2 = getgenpept('NP_536843', 'SequenceOnly', true)
```

The following example converts the gene ND2 on the human mitochondria genome to an amino acid sequence. In this case, the first codon is ATT, which is translated to M, while the following ATT codons are converted to I. If you set 'AlternativeStartCodons' to `false`, then the first codon ATT is translated to I, the corresponding amino acid in the Vertebrate Mitochondrial genetic code.

```
mitochondria = getgenbank('NC_001807', 'SequenceOnly', true)
ND2gene = mitochondria (4471:5514)
protein1 = nt2aa(ND2gene, 'GeneticCode', 2)
protein2 = getgenpept('NP_536844', 'SequenceOnly', true)
```

See Also

Bioinformatics Toolbox functions: aa2int, aminolookup, baselookup, codonbias, dnds, dndsml, geneticcode, revgeneticcode, seqtool

nt2int

Purpose

Convert nucleotide sequence from letter to integer representation

Syntax

```
SeqInt = nt2int(SeqChar, 'PropertyName', PropertyValue)
nt2int(..., 'Unknown', UnknownValue)
nt2int(..., 'ACGTOnly', ACGTONlyValue)
```

Arguments

`SeqChar`	Nucleotide sequence represented with letters. Enter a character string from the table Mapping Nucleotide Letters to Integers below. Integers are arbitrarily assigned to IUB/IUPAC letters. If the property `ACGTOnly` is `true`, you can only enter the characters `A`, `C`, `T`, `G`, and `U`.
`UnknownValue`	Property to select the integer for unknown characters. Enter an integer. Maximum value is `255`. Default value is `0`.
`ACGTOnlyValue`	Property to control the use of ambiguous nucleotides. Enter either `true` or `false`. Default value is `false`.

Mapping Nucleotide Letters to Integers

Base	Code	Base	Code	Base	Code
Adenosine	A—1	T, C (pyrimidine)	Y—6	A, T, G (not C)	D—12
Cytidine	C—2	G, T (keto)	K—7	A, T, C (not G)	H—13
Guanine	G—3	A, C (amino)	M—8	A, G, C (not T)	V—14
Thymidine	T—4	G, C (strong)	S—9	A, T, G, C (any)	N—15

Base	Code	Base	Code	Base	Code
Uridine	U—4	A, T (weak)	W—10	Gap of indeterminate length	- —16
A, G (purine)	R—5	T, G, C (not A)	B—11	Unknown (default)	*—0 and ≥17

Description

SeqInt = nt2int(SeqChar, '*PropertyName*', *PropertyValue*) converts a character string of nucleotides to a 1-by-N array of integers using the table Mapping Nucleotide Letters to Integers above. Unknown characters (characters not in the table) are mapped to 0. Gaps represented with hyphens are mapped to 16.

nt2int(..., 'Unknown', *UnknownValue*) defines the number used to represent unknown nucleotides. The default value is 0.

nt2int(..., 'ACGTOnly', *ACGTONlyValue*) if ACGTOnly is true, the ambiguous nucleotide characters (N, R, Y, K, M, S, W, B, D, H, and V) are represented by the unknown nucleotide number.

Examples

Convert a nucleotide sequence with letters to integers.

```
s = nt2int('ACTGCTAGC')

s =
     1     2     4     3     2     4     1     3     2
```

See Also

Bioinformatics Toolbox functions: aa2int, baselookup, int2aa, int2nt

ntdensity

Purpose Plot density of nucleotides along sequence

Syntax

```
Density = ntdensity(SeqNT, 'PropertyName', PropertyValue)
ntdensity(..., 'Window', WindowValue)
[Density, HighCG] = ntdensity(..., 'CGThreshold',
   CGThresholdValue)
```

Description

`ntdensity(SeqNT)` plots the density of nucleotides `A`, `T`, `C`, `G` in sequence `SeqNT`.

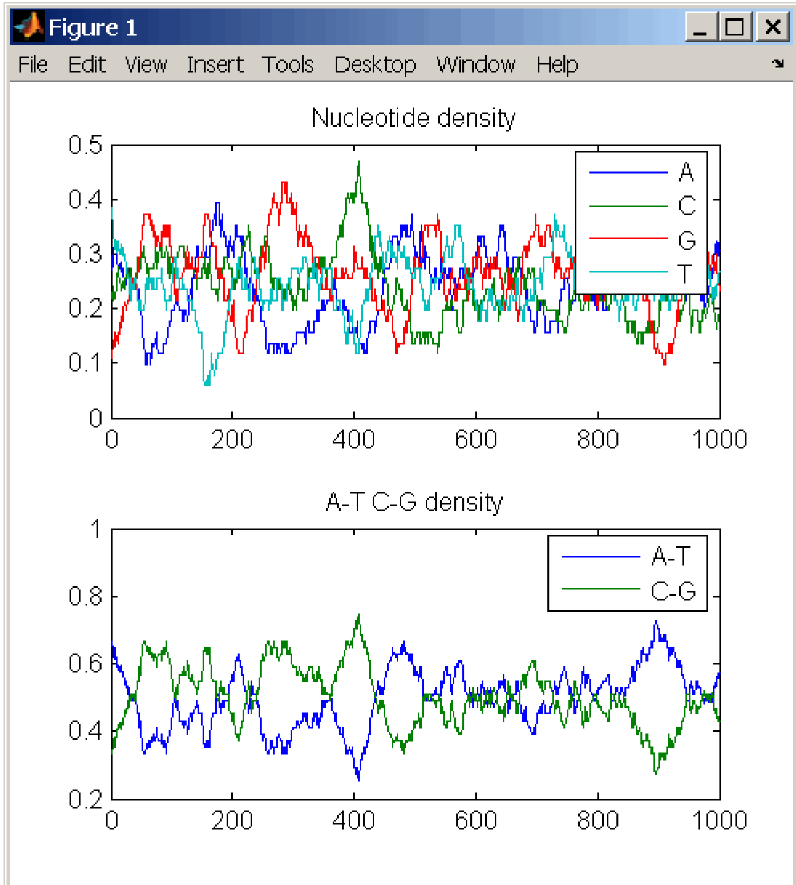
`Density = ntdensity(SeqNT, 'PropertyName', PropertyValue)` returns a MATLAB structure with the density of nucleotides `A`, `C`, `G`, and `T`.

`ntdensity(..., 'Window', WindowValue)` uses a window of length `Window` for the density calculation. The default value is `length(SeqNT)/20`.

`[Density, HighCG] = ntdensity(..., 'CGThreshold', CGThresholdValue)` returns indices for regions where the `CG` content of `SeqNT` is greater than `CGThreshold`. The default value for `CGThreshold` is `5`.

Examples

```
s = randseq(1000, 'alphabet', 'dna');
ndensity(s)
```



See Also

Bioinformatics Toolbox functions `basecount`, `codoncount`, `cpgisland`, `dimercount`

MATLAB function `filter`

Purpose NUC44 scoring matrix for nucleotide sequences

Syntax

```
ScoringMatrix = nuc44
[ScoringMatrix, MatrixInfo] = nuc44
```

Description *ScoringMatrix* = nuc44 returns the scoring matrix. The nuc44 scoring matrix uses ambiguous nucleotide codes and probabilities rounded to the nearest integer.

Scale = 0.277316

Expected score = -1.7495024, Entropy = 0.5164710 bits

Lowest score = -4, Highest score = 5

Order: A C G T R Y K M S W B D H V N

[*ScoringMatrix*, *MatrixInfo*] = nuc44 returns a structure with information about the matrix with fields Name and Order.

Purpose

Convert numbers to Gene Ontology IDs

Syntax

GOIDs = num2goid(*X*)

Description

GOIDs = num2goid(*X*) converts the numbers in *X* to strings with Gene Ontology IDs. IDs are a 7-digit number preceded by the prefix 'GO:'.

Examples

Get the Gene Ontology IDs of the following numbers.

```
t = [5575 5622 5623 5737 5840 30529 43226 43228 ...
     43229 43232 43234];
ids = num2goid(t)
```

See Also

Bioinformatics Toolbox functions: geneont (object constructor), goannotread

Bioinformatics Toolbox methods of geneont object: getancestors, getdescendants, getmatrix, getrelatives

nwalign

Purpose

Globally align two sequences using Needleman-Wunsch algorithm

Syntax

```
Score = nwalign(Seq1,Seq2)
[Score, Alignment] = nwalign(Seq1,Seq2)
[Score, Alignment, Start] = nwalign(Seq1,Seq2)
... = nwalign(Seq1,Seq2, ...'Alphabet', AlphabetValue, ...)
... = nwalign(Seq1,Seq2, ...'ScoringMatrix',
    ScoringMatrixValue, ...)
... = nwalign(Seq1,Seq2, ...'Scale', ScaleValue, ...)
... = nwalign(Seq1,Seq2, ...'GapOpen', GapOpenValue, ...)
... = nwalign(Seq1,Seq2, ...'ExtendGap',
ExtendGapValue, ...)
... = nwalign(Seq1,Seq2, ...'Showscore',
ShowscoreValue, ...)
```

Arguments

Seq1, *Seq2*

Amino acid or nucleotide sequences. Enter any of the following:

- Character string of letters representing amino acids or nucleotides, such as returned by `int2aa` or `int2nt`
- Vector of integers representing amino acids or nucleotides, such as returned by `aa2int` or `nt2int`
- Structure containing a `Sequence` field

Tip For help with letter and integer representations of amino acids and nucleotides, see Amino Acid Lookup Table on page 2-42 or Nucleotide Lookup Table on page 2-52.

AlphabetValue

String specifying the type of sequence. Choices are `'AA'` (default) or `'NT'`.

ScoringMatrixValue	String specifying the scoring matrix to use for the global alignment. Choices for amino acid sequences are: • `'PAM40'` • `'PAM250'` • `'DAYHOFF'` • `'GONNET'` • `'BLOSUM30'` increasing by `5` up to `'BLOSUM90'` • `'BLOSUM62'` • `'BLOSUM100'` Default is: • `'BLOSUM50'` (when *AlphabetValue* equals `'AA'`) • `'NUC44'` (when *AlphabetValue* equals `'NT'`) **Note** All of the above scoring matrices have a built-in scale factor that returns *Score* in bits.
ScaleValue	Positive value that specifies the scale factor used to return *Score* in arbitrary units other than bits. For example, if you enter `log(2)` for *ScaleValue*, then `nwalign` returns *Score* in nats.
GapOpenValue	Positive integer specifying the penalty for opening a gap in the alignment. Default is `8`.

ExtendGapValue	Positive integer specifying the penalty for extending a gap. Default is equal to *GapOpenValue*.
ShowscoreValue	Controls the display of the scoring space and the winning path of the alignment. Choices are `true` or `false` (default).

Return Values

Score	Optimal global alignment score in bits.
Alignment	3-by-N character array showing the two sequences, *Seq1* and *Seq2*, in the first and third rows, and symbols representing the optimal global alignment for them in the second row.
Start	2-by-1 vector of indices indicating the starting point in each sequence for the alignment. Because this is a global alignment, *Start* is always `[1;1]`.

Description

`Score = nwalign(Seq1,Seq2)` returns the optimal global alignment score in bits. The scale factor used to calculate the score is provided by the scoring matrix.

`[Score, Alignment] = nwalign(Seq1,Seq2)` returns a 3-by-N character array showing the two sequences, *Seq1* and *Seq2*, in the first and third rows, and symbols representing the optimal global alignment for them in the second row. The symbol `|` indicates amino acids or nucleotides that match exactly. The symbol `:` indicates amino acids or nucleotides that are related as defined by the scoring matrix (nonmatches with a zero or positive scoring matrix value).

`[Score, Alignment, Start] = nwalign(Seq1,Seq2)` returns a 2-by-1 vector of indices indicating the starting point in each sequence for the alignment. Because this is a global alignment, *Start* is always `[1;1]`.

`... = nwalign(`*`Seq1`*`,`*`Seq2`*`, ...'`*`PropertyName`*`',` *`PropertyValue`*`, ...)` calls `nwalign` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = nwalign(`*`Seq1`*`,`*`Seq2`*`, ...'Alphabet',` *`AlphabetValue`*`, ...)` specifies the type of sequences. Choices are `'AA'` (default) or `'NT'`.

`... = nwalign(`*`Seq1`*`,`*`Seq2`*`, ...'ScoringMatrix',` *`ScoringMatrixValue`*`, ...)` specifies the scoring matrix to use for the global alignment. Default is:

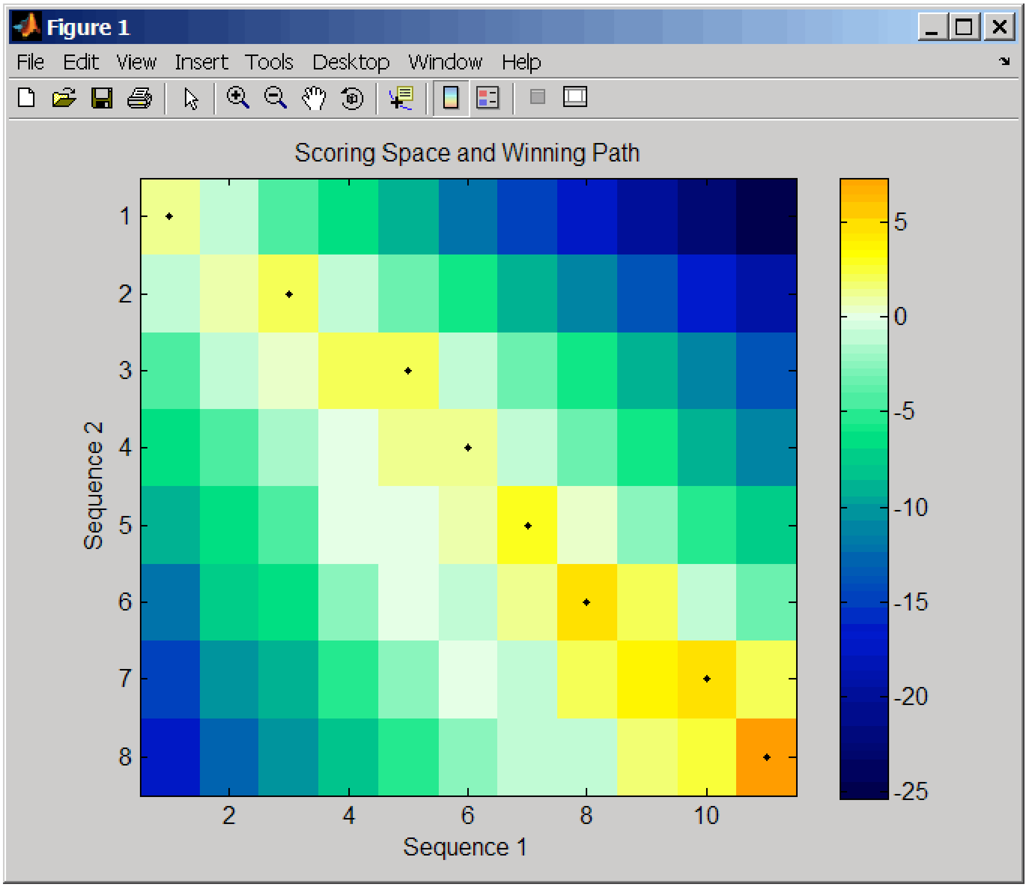
- `'BLOSUM50'` (when *`AlphabetValue`* equals `'AA'`)
- `'NUC44'` (when *`AlphabetValue`* equals `'NT'`)

`... = nwalign(`*`Seq1`*`,`*`Seq2`*`, ...'Scale',` *`ScaleValue`*`, ...)` specifies the scale factor used to return *`Score`* in arbitrary units other than bits. Choices are any positive value.

`... = nwalign(`*`Seq1`*`,`*`Seq2`*`, ...'GapOpen',` *`GapOpenValue`*`, ...)` specifies the penalty for opening a gap in the alignment. Choices are any positive integer. Default is `8`.

`... = nwalign(`*`Seq1`*`,`*`Seq2`*`, ...'ExtendGap',` *`ExtendGapValue`*`, ...)` specifies the penalty for extending a gap in the alignment. Choices are any positive integer. Default is equal to *`GapOpenValue`*.

`... = nwalign(`*`Seq1`*`,`*`Seq2`*`, ...'Showscore',` *`ShowscoreValue`*`, ...)` controls the display of the scoring space and winning path of the alignment. Choices are `true` or `false` (default)



The scoring space is a heat map displaying the best scores for all the partial alignments of two sequences. The color of each (`n1,n2`) coordinate in the scoring space represents the best score for the pairing of subsequences `Seq1(1:n1)` and `Seq2(1:n2)`, where `n1` is a position in `Seq1` and `n2` is a position in `Seq2`. The best score for a pairing of specific subsequences is determined by scoring all possible alignments of the subsequences by summing matches and gap penalties.

The winning path is represented by black dots in the scoring space and represents the pairing of positions in the optimal global alignment. The color of the last point (lower right) of the winning path represents the optimal global alignment score for the two sequences and is the *Score* output returned by `nwalign`.

Tip The scoring space visually indicates if there are potential alternate winning paths, which is useful when aligning sequences with big gaps. Visual patterns in the scoring space can also indicate a possible sequence rearrangement.

Examples

1. Globally align two amino acid sequences using the `BLOSUM50` (default) scoring matrix and the default values for the `GapOpen` and `ExtendGap` properties. Return the optimal global alignment score in bits and the alignment character array.

```
[Score, Alignment] = nwalign('VSPAGMASGYD','IPGKASYD')

Score =

    7.3333

Alignment =

VSPAGMASGYD
: | | || ||
I-P-GKAS-YD
```

2. Globally align two amino acid sequences specifying the `PAM250` scoring matrix and a gap open penalty of `5`.

```
[Score, Alignment] = nwalign('IGRHRYHIGG','SRYIGRG',...
                             'scoringmatrix','pam250',...
                             'gapopen',5)
```

```
Score =

    2.3333

Alignment =

IGRHRYHIG-G
 :  || || |
-S--RY-IGRG
```

3 Globally align two amino acid sequences returning the *Score* in nat units (nats) by specifying a scale factor of `log(2)`.

```
[Score, Alignment] = nwalign('HEAGAWGHEE','PAWHEAE','Scale',log(2))

Score =

    0.2310

Alignment =

HEAGAWGHE-E
    || || |
--P-AW-HEAE
```

References

[1] Durbin, R., Eddy, S., Krogh, A., and Mitchison, G. (1998). Biological Sequence Analysis (Cambridge University Press).

See Also

Bioinformatics Toolbox functions: `blosum`, `multialign`, `nt2aa`, `pam`, `profalign`, `seqdotplot`, `showalignment`, `swalign`

Purpose

Calculate sequence properties of DNA oligonucleotide

Syntax

```
SeqProperties = oligoprop(SeqNT)
SeqProperties = oligoprop(SeqNT, ...'Salt', SaltValue, ...)
SeqProperties = oligoprop(SeqNT, ...'Temp', TempValue, ...)
SeqProperties = oligoprop(SeqNT, ...'Primerconc',
   PrimerconcValue, ...)
SeqProperties = oligoprop(SeqNT, ...'HPBase', HPBaseValue,
   ...)
SeqProperties = oligoprop(SeqNT, ...'HPLoop', HPLoopValue,
   ...)
SeqProperties = oligoprop(SeqNT, ...'Dimerlength',
   DimerlengthValue, ...)
```

Arguments

SeqNT	DNA oligonucleotide sequence represented by any of the following: • Character string containing the letters A, C, G, T, or N • Vector of integers containing the integers 1, 2, 3, 4, or 15 • Structure containing a Sequence field that contains a nucleotide sequence
SaltValue	Value that specifies a salt concentration in moles/liter for melting temperature calculations. Default is 0.05 moles/liter.
TempValue	Value that specifies the temperature in degrees Celsius for nearest-neighbor calculations of free energy. Default is 25 degrees Celsius.
PrimerconcValue	Value that specifies the concentration in moles/liter for melting temperature calculations. Default is 50e-6 moles/liter.

HPBaseValue	Value that specifies the minimum number of paired bases that form the neck of the hairpin. Default is `4` base pairs.
HPLoopValue	Value that specifies the minimum number of bases that form the loop of a hairpin. Default is `2` bases.
DimerlengthValue	Value that specifies the minimum number of aligned bases between the sequence and its reverse. Default is `4` bases.

Return Values

SeqProperties	Structure containing the sequence properties for a DNA oligonucleotide.

Description

SeqProperties = `oligoprop(`*SeqNT*`)` returns the sequence properties for a DNA oligonucleotide as a structure with the following fields:

Field	Description
`GC`	Percent GC content for the DNA oligonucleotide. Ambiguous `N` characters in *SeqNT* are considered to potentially be any nucleotide. If *SeqNT* contains ambiguous `N` characters, `GC` is the midpoint value, and its uncertainty is expressed by `GCdelta`.
`GCdelta`	The difference between `GC` (midpoint value) and either the maximum or minimum value `GC` could assume. The maximum and minimum values are calculated by assuming all `N` characters are G/C or not G/C, respectively. Therefore, `GCdelta` defines the possible range of GC content.

Field	Description
`Hairpins`	`H`-by-`length(`*SeqNT*`)` matrix of characters displaying all potential hairpin structures for the sequence *SeqNT*. Each row is a potential hairpin structure of the sequence, with the hairpin forming nucleotides designated by capital letters. `H` is the number of potential hairpin structures for the sequence. Ambiguous `N` characters in *SeqNT* are considered to potentially complement any nucleotide.
`Dimers`	`D`-by-`length(`*SeqNT*`)` matrix of characters displaying all potential dimers for the sequence *SeqNT*. Each row is a potential dimer of the sequence, with the self-dimerizing nucleotides designated by capital letters. `D` is the number of potential dimers for the sequence. Ambiguous `N` characters in *SeqNT* are considered to potentially complement any nucleotide.
`MolWeight`	Molecular weight of the DNA oligonucleotide. Ambiguous `N` characters in *SeqNT* are considered to potentially be any nucleotide. If *SeqNT* contains ambiguous `N` characters, `MolWeight` is the midpoint value, and its uncertainty is expressed by `MolWeightdelta`.
`MolWeightdelta`	The difference between `MolWeight` (midpoint value) and either the maximum or minimum value `MolWeight` could assume. The maximum and minimum values are calculated by assuming all `N` characters are `G` or `C`, respectively. Therefore, `MolWeightdelta` defines the possible range of molecular weight for *SeqNT*.

Field	Description
`Tm`	A vector with melting temperature values, in degrees Celsius, calculated by six different methods, listed in the following order: • Basic (Marmur et al., 1962) • Salt adjusted (Howley et al., 1979) • Nearest-neighbor (Breslauer et al., 1986) • Nearest-neighbor (SantaLucia Jr. et al., 1996) • Nearest-neighbor (SantaLucia Jr., 1998) • Nearest-neighbor (Sugimoto et al., 1996) Ambiguous `N` characters in *`SeqNT`* are considered to potentially be any nucleotide. If *`SeqNT`* contains ambiguous `N` characters, `Tm` is the midpoint value, and its uncertainty is expressed by `Tmdelta`.
`Tmdelta`	A vector containing the differences between `Tm` (midpoint value) and either the maximum or minimum value `Tm` could assume for each of the six methods. Therefore, `Tmdelta` defines the possible range of melting temperatures for *`SeqNT`*.

Field	Description
`Thermo`	4-by-3 matrix of thermodynamic calculations. The rows correspond to nearest-neighbor parameters from: • Breslauer et al., 1986 • SantaLucia Jr. et al., 1996 • SantaLucia Jr., 1998 • Sugimoto et al., 1996 The columns correspond to: • delta `H` — Enthalpy in kilocalories per mole, kcal/mol • delta `S` — Entropy in calories per mole-degrees Kelvin, cal/(K)(mol) • delta `G` — Free energy in kilocalories per mole, kcal/mol Ambiguous `N` characters in *`SeqNT`* are considered to potentially be any nucleotide. If *`SeqNT`* contains ambiguous `N` characters, `Thermo` is the midpoint value, and its uncertainty is expressed by `Thermodelta`.
`Thermodelta`	4-by-3 matrix containing the differences between `Thermo` (midpoint value) and either the maximum or minimum value `Thermo` could assume for each calculation and method. Therefore, `Thermodelta` defines the possible range of thermodynamic values for *`SeqNT`*.

`SeqProperties` `= oligoprop(`*`SeqNT`*`, ...'`*`PropertyName`*`',` *`PropertyValue`*`, ...)` calls `oligoprop` with optional properties that

use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

SeqProperties = oligoprop(*SeqNT*, ...'Salt', *SaltValue*, ...) specifies a salt concentration in moles/liter for melting temperature calculations. Default is 0.05 moles/liter.

SeqProperties = oligoprop(*SeqNT*, ...'Temp', *TempValue*, ...) specifies the temperature in degrees Celsius for nearest-neighbor calculations of free energy. Default is 25 degrees Celsius.

SeqProperties = oligoprop(*SeqNT*, ...'Primerconc', *PrimerconcValue*, ...) specifies the concentration in moles/liter for melting temperatures. Default is 50e-6 moles/liter.

SeqProperties = oligoprop(*SeqNT*, ...'HPBase', *HPBaseValue*, ...) specifies the minimum number of paired bases that form the neck of the hairpin. Default is 4 base pairs.

SeqProperties = oligoprop(*SeqNT*, ...'HPLoop', *HPLoopValue*, ...) specifies the minimum number of bases that form the loop of a hairpin. Default is 2 bases.

SeqProperties = oligoprop(*SeqNT*, ...'Dimerlength', *DimerlengthValue*, ...) specifies the minimum number of aligned bases between the sequence and its reverse. Default is 4 bases.

Examples

Calculating Properties for a DNA Sequence

1 Create a random sequence.

```
seq = randseq(25)

seq =

TAGCTTCATCGTTGACTTCTACTAA
```

2 Calculate sequence properties of the sequence.

```
S1 = oligoprop(seq)

S1 =

              GC: 36
         GCAlpha: 0
        Hairpins: [0x25 char]
          Dimers: 'tAGCTtcatcgttgacttctactaa'
       MolWeight: 7.5820e+003
  MolWeightAlpha: 0
              Tm: [52.7640 60.8629 62.2493 55.2870 54.0293 61.0614]
         TmAlpha: [0 0 0 0 0 0]
          Thermo: [4x3 double]
     ThermoAlpha: [4x3 double]
```

3 List the thermodynamic calculations for the sequence.

```
S1.Thermo

ans =

 -178.5000 -477.5700  -36.1125
 -182.1000 -497.8000  -33.6809
 -190.2000 -522.9000  -34.2974
 -191.9000 -516.9000  -37.7863
```

Calculating Properties for a DNA Sequence with Ambiguous Characters

1 Calculate sequence properties of the sequence ACGTAGAGGACGTN.

```
S2 = oligoprop('ACGTAGAGGACGTN')

S2 =

              GC: 53.5714
         GCAlpha: 3.5714
        Hairpins: 'ACGTagaggACGTn'
```

```
          Dimers: [3x14 char]
       MolWeight: 4.3329e+003
  MolWeightAlpha: 20.0150
              Tm: [38.8357 42.2958 57.7880 52.4180 49.9633 55.1330]
         TmAlpha: [1.4643 1.4643 10.3885 3.4633 0.2829 3.8074]
          Thermo: [4x3 double]
     ThermoAlpha: [4x3 double]
```

2 List the potential dimers for the sequence.

```
S2.Dimers

ans =

ACGTagaggacgtn
ACGTagaggACGTn
acgtagagGACGTN
```

References

[1] Breslauer, K.J., Frank, R., Blöcker, H., and Marky, L.A. (1986). Predicting DNA duplex stability from the base sequence. Proceedings of the National Academy of Science USA *83*, 3746–3750.

[2] Chen, S.H., Lin, C.Y., Cho, C.S., Lo, C.Z., and Hsiung, C.A. (2003). Primer Design Assistant (PDA): A web-based primer design tool. Nucleic Acids Research *31(13)*, 3751–3754.

[3] Howley, P.M., Israel, M.A., Law, M., and Martin, M.A. (1979). A rapid method for detecting and mapping homology between heterologous DNAs. Evaluation of polyomavirus genomes. The Journal of Biological Chemistry *254(11)*, 4876–4883.

[4] Marmur, J., and Doty, P. (1962). Determination of the base composition of deoxyribonucleic acid from its thermal denaturation temperature. Journal Molecular Biology *5*, 109–118.

[5] Panjkovich, A., and Melo, F. (2005). Comparison of different melting temperature calculation methods for short DNA sequences. Bioinformatics *21(6)*, 711–722.

[6] SantaLucia Jr., J., Allawi, H.T., and Seneviratne, P.A. (1996). Improved Nearest-Neighbor Parameters for Predicting DNA Duplex Stability. Biochemistry *35*, 3555–3562.

[7] SantaLucia Jr., J. (1998). A unified view of polymer, dumbbell, and oligonucleotide DNA nearest-neighbor thermodynamics. Proceedings of the National Academy of Science USA *95*, 1460–1465.

[8] Sugimoto, N., Nakano, S., Yoneyama, M., and Honda, K. (1996). Improved thermodynamic parameters and helix initiation factor to predict stability of DNA duplexes. Nucleic Acids Research *24(22)*, 4501–4505.

[9] http://www.basic.northwestern.edu/biotools/oligocalc.html for weight calculations.

See Also

Bioinformatics Toolbox functions: `isoelectric`, `molweight`, `ntdensity`, `palindromes`, `randseq`

Purpose Determine optimal leaf ordering for hierarchical binary cluster tree

Syntax

```
Order = optimalleaforder(Tree, Dist)
Order = optimalleaforder(Tree, Dist, ...'Criteria',
CriteriaValue, ...)
Order = optimalleaforder(Tree, Dist, ...'Transformation',
   TransformationValue, ...)
```

Arguments

Tree	Hierarchical binary cluster tree represented by an (M - 1)-by-3 matrix, created by the `linkage` function, where M is the number of leaves.
Dist	Distance matrix, such as that created by the `pdist` function.

CriteriaValue	String that specifies the optimization criteria. Choices are: • adjacent (default) — Minimizes the sum of distances between adjacent leaves. • group — Minimizes the sum of distances between every leaf and all other leaves in the adjacent cluster.
TransformationValue	Either of the following: • String that specifies the algorithm to transform the distances in *Dist* into similarity values. Choices are: - linear (default) — Similarity = max(all distances) - distance - quadratic — Similarity = (max(all distances) - distance)^2 - inverse — Similarity = 1/distance • A function handle created using @ to a function that transforms the distances in *Dist* into similarity values. The function is typically a monotonic decreasing function within the range of the distance values. The function must accept a vector input and return a vector of the same size.

Return Values

Order	Optimal leaf ordering for the hierarchical binary cluster tree represented by *Tree*.

Description

Order = optimalleaforder(*Tree*, *Dist*) returns the optimal leaf ordering for the hierarchical binary cluster tree represented by *Tree*, an (M - 1)-by-3 matrix, created by the linkage function, where M is the number of leaves. Optimal leaf ordering of a binary tree maximizes the similarity between adjacent elements (clusters or leaves) by flipping tree branches, but without dividing the clusters. The input *Dist* is a distance matrix, such as that created by the `pdist` function.

Order = `optimalleaforder(`*Tree*`,` *Dist*`, ...'`*PropertyName*`',` *PropertyValue*`, ...)` calls `optimalleaforder` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

Order = `optimalleaforder(`*Tree*`,` *Dist*`, ...'Criteria',` *CriteriaValue*`, ...)` specifies the optimization criteria.

Order = `optimalleaforder(`*Tree*`,` *Dist*`, ...'Transformation',` *TransformationValue*`, ...)` specifies the algorithm to transform the distances in *Dist* into similarity values. The transformation is necessary because `optimalleaforder` maximizes the similarity between adjacent elements, which is comparable to minimizing the sum of distances between adjacent elements.

Examples

1. Use the `rand` function to create a 10-by-2 matrix of random values.

   ```
   X = rand(10,2);
   ```

2. Use the `pdist` function to create a distance matrix containing the city block distances between the pairs of objects in matrix `X`.

   ```
   Dist = pdist(X,'cityblock');
   ```

3. Use the `linkage` function to create a matrix, `Tree`, that represents a hierarchical binary cluster tree, from the distance matrix, `Dist`.

   ```
   Tree = linkage(Dist,'average');
   ```

4. Use the `optimalleaforder` function to determine the optimal leaf ordering for the hierarchical binary cluster tree represented by `Tree`, using the distance matrix `Dist`.

   ```
   order = optimalleaforder(Tree,Dist)
   ```

References

[1] Bar-Joseph, Z., Gifford, D.K., and Jaakkola, T.S. (2001). Fast optimal leaf ordering for hierarchical clustering. Bioinformatics *17*, Suppl 1:S22–9. PMID: 11472989.

See Also

Bioinformatics Toolbox function: `clustergram`

Statistics Toolbox functions: `linkage`, `pdist`

palindromes

Purpose

Find palindromes in sequence

Syntax

```
[Position, Length] = palindromes(SeqNT, 'PropertyName',
   PropertyValue)
[Position, Length, Pal] = palindromes(SeqNT)
palindromes(..., 'Length',LengthValue)
palindromes(..., 'Complement', ComplementValue)
```

Description

`[Position, Length] = palindromes(SeqNT, 'PropertyName', PropertyValue)` finds all palindromes in sequence `SeqNT` with a length greater than or equal to `6`, and returns the starting indices, `Position`, and the lengths of the palindromes, `Length`.

`[Position, Length, Pal] = palindromes(SeqNT)` also returns a cell array `Pal` of the palindromes.

`palindromes(..., 'Length',LengthValue)` finds all palindromes longer than or equal to `Length`. The default value is `6`.

`palindromes(..., 'Complement', ComplementValue)` finds complementary palindromes if `Complement` is `true`, that is, where the elements match their complementary pairs `A-T`(or `U`) and `C-G` instead of an exact nucleotide match.

Examples

```
[p,l,s] = palindromes('GCTAGTAACGTATATATAAT')

p =
    11
    12
l =
     7
     7
s =
    'TATATAT'
    'ATATATA'

[pc,lc,sc] = palindromes('GCTAGTAACGTATATATAAT',...
                         'Complement',true);
```

Find the palindromes in a random nucleotide sequence.

```
a = randseq(100)

a =
TAGCTTCATCGTTGACTTCTACTAA
AAGCAAGCTCCTGAGTAGCTGGCCA
AGCGAGCTTGCTTGTGCCCGGCTGC
GGCGGTTGTATCCTGAATACGCCAT

[pos,len,pal]=palindromes(a)

pos =
    74
len =
     6
pal =
    'GCGGCG'
```

See Also

Bioinformatics Toolbox functions `seqrcomplement`, `seqshowwords`

MATLAB functions `regexp`, `strfind`

Purpose

PAM scoring matrix

Syntax

```
ScoringMatrix = pam(N, 'PropertyName', PropertyValue)
[ScoringMatrix, MatrixInfo] = pam(N)
ScoringMatrix = pam(..., 'Extended', 'ExtendedValue')
ScoringMatrix = pam(..., 'Order', 'OrderValue')
```

Arguments

`N`	Enter values `10:10:500`. The default ordering of the output is `A R N D C Q E G H I L K M F P S T W Y V B Z X *`. Entering a larger value for N to allow sequence alignments with larger evolutionary distances.
`Extended`	Property to add ambiguous characters to the scoring matrix. Enter either `true` or `false`. Default is `false`.
`Order`	Property to control the order of amino acids in the scoring matrix. Enter a string with at least the 20 standard amino acids.

Description

`ScoringMatrix = pam(N, 'PropertyName', PropertyValue)` returns a PAM scoring matrix for amino acid sequences.

`[ScoringMatrix, MatrixInfo] = pam(N)` returns a structure with information about the PAM matrix. The fields in the structure are `Name`, `Scale`, `Entropy`, `Expected`, and `Order`.

`ScoringMatrix = pam(..., 'Extended', 'ExtendedValue')` if `Extended` is `true`, returns a scoring matrix with the 20 amino acid characters, the ambiguous characters, and stop character (`B`, `Z`, `X`, `*`), . If `Extended` is `false`, only the standard 20 amino acids are included in the matrix.

`ScoringMatrix = pam(..., 'Order', 'OrderValue')` returns a PAM matrix ordered by the amino acid sequence in `Order`. If `Order` does not contain the extended characters `B`, `Z`, `X`, and `*`, then these characters are not returned.

PAM50 substitution matrix in 1/2 bit units, Expected score = -3.70, Entropy = 2.00 bits, Lowest score = -13, Highest score = 13.

PAM250 substitution matrix in 1/3 bit units, Expected score = -0.844, Entropy = 0.354 bits, Lowest score = -8, Highest score = 17.

Examples

Get the PAM matrix with N = 50.

```
PAM50 = pam(50)

PAM250 = pam(250,'Order','CSTPAGNDEQHRKMILVFYW')
```

See Also

Bioinformatics Toolbox functions blosum, dayhoff, gonnet, nwalign, swalign

pdbdistplot

Purpose

Visualize intermolecular distances in Protein Data Bank (PDB) file

Syntax

```
pdbdistplot('PDBid')
pdbdistplot('PDBid', Distance)
```

Arguments

`PDBid`	Unique identifier for a protein structure record. Each structure in the PDB is represented by a 4-character alphanumeric identifier. For example, `4hhb` is the identification code for hemoglobin.
`Distance`	Threshold distance in Angstroms shown on a spy plot. Default value is `7`.

Description

`pdbdistplot` displays the distances between atoms and amino acids in a PDB structure.

`pdbdistplot('PDBid')` retrieves the entry `PDBid` from the Protein Data Bank (PDB) database and creates a heat map showing interatom distances and a spy plot showing the residues where the minimum distances apart are less than `7` Angstroms. `PDBid` can also be the name of a variable or a file containing a PDB MATLAB structure.

`pdbdistplot('PDBid', Distance)` specifies the threshold distance shown on a spy plot.

Examples

Show spy plot at `7` Angstroms of the protein cytochrome C from albacore tuna.

```
pdbdistplot('5CYT');
```

Now take a look at `10` Angstroms.

```
pdbdistplot('5CYT',10);
```

See Also

Bioinformatics Toolbox functions: `getpdb`, `molviewer`, `pdbread`, `proteinplot`, `ramachandran`

pdbread

Purpose

Read data from Protein Data Bank (PDB) file

Syntax

```
PDBStruct = pdbread(File)
PDBStruct = pdbread(File, 'ModelNum', ModelNumValue)
```

Arguments

File	Either of the following: • String specifying a file name, a path and file name, or a URL pointing to a file. The referenced file is a Protein Data Bank (PDB)-formatted file (ASCII text file). If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Directory. • MATLAB character array that contains the text of a PDB-formatted file.
ModelNumValue	Positive integer specifying a model in a PDB-formatted file.

Return Values

PDBStruct	MATLAB structure containing a field for each PDB record.

Description

The Protein Data Bank (PDB) database is an archive of experimentally determined 3-D biological macromolecular structure data. For more information about the PDB format, see:

```
http://www.rcsb.org/pdb/file_formats/pdb/pdbguide2.2/guide2.2_frame.html
```

PDBStruct = pdbread(*File*) reads the data from PDB-formatted text file *File* and stores the data in the MATLAB structure, *PDBStruct*, which contains a field for each PDB record. The following table summarizes the possible PDB records and the corresponding fields in the MATLAB structure *PDBStruct*:

PDB Database Record	Field in the MATLAB Structure
HEADER	Header
OBSLTE	Obsolete
TITLE	Title
CAVEAT	Caveat
COMPND	Compound
SOURCE	Source
KEYWDS	Keywords
EXPDTA	ExperimentData
AUTHOR	Authors
REVDAT	RevisionDate
SPRSDE	Superseded
JRNL	Journal
REMARK 1	Remark1
REMARK *N* **Note** N equals 2 through 999.	Remark*n* **Note** n equals 2 through 999.
DBREF	DBReferences
SEQADV	SequenceConflicts
SEQRES	Sequence
FTNOTE	Footnote
MODRES	ModifiedResidues

PDB Database Record	Field in the MATLAB Structure
HET	Heterogen
HETNAM	HeterogenName
HETSYN	HeterogenSynonym
FORMUL	Formula
HELIX	Helix
SHEET	Sheet
TURN	Turn
SSBOND	SSBond
LINK	Link
HYDBND	HydrogenBond
SLTBRG	SaltBridge
CISPEP	CISPeptides
SITE	Site
CRYST1	Cryst1
ORIGXn	OriginX
SCALEn	Scale
MTRIXn	Matrix
TVECT	TranslationVector
MODEL	Model
ATOM	Atom
SIGATM	AtomSD
ANISOU	AnisotropicTemp
SIGUIJ	AnisotropicTempSD
TER	Terminal

PDB Database Record	Field in the MATLAB Structure
HETATM	HeterogenAtom
CONECT	Connectivity

PDBStruct = pdbread(*File*, 'ModelNum', *ModelNumValue*) reads only the model specified by *ModelNumValue* from the PDB-formatted text file *File* and stores the data in the MATLAB structure *PDBStruct*. If *ModelNumValue* does not correspond to an existing mode number in *File*, then pdbread reads the coordinate information of all the models.

The Sequence Field

The Sequence field is also a structure containing sequence information in the following subfields:

- NumOfResidues
- ChainID
- ResidueNames — Contains the three-letter codes for the sequence residues.
- Sequence — Contains the single-letter codes for the sequence residues.

Note If the sequence has modified residues, then the ResidueNames subfield might not correspond to the standard three-letter amino acid codes. In this case, the Sequence subfield will contain the modified residue code in the position corresponding to the modified residue. The modified residue code is provided in the ModifiedResidues field.

The Model Field

The Model field is also a structure or an array of structures containing coordinate information. If the MATLAB structure contains one model, the Model field is a structure containing coordinate information for that model. If the MATLAB structure contains multiple models, the Model field is an array of structures containing coordinate information for each model. The `Model` field contains the following subfields:

- `Atom`
- `AtomSD`
- `AnisotropicTemp`
- `AnisotropicTempSD`
- `Terminal`
- `HeterogenAtom`

The Atom Field

The `Atom` field is also an array of structures containing the following subfields:

- `AtomSerNo`
- `AtomName`
- `altLoc`
- `resName`
- `chainID`
- `resSeq`
- `iCode`
- `X`
- `Y`
- `Z`
- `occupancy`
- `tempFactor`
- `segID`
- `element`

- `charge`
- `AtomNameStruct` — Contains three subfields: `chemSymbol`, `remoteInd`, and `branch`.

Examples

1 Use the `getpdb` function to retrieve structure information from the Protein Data Bank (PDB) for the nicotinic receptor protein with identifier `1abt`, and then save the data to the PDB-formatted file `nicotinic_receptor.pdb` in the MATLAB Current Directory.

```
getpdb('1abt', 'ToFile', 'nicotinic_receptor.pdb');
```

2 Read the data from the `nicotinic_receptor.pdb` file into a MATLAB structure `pdbstruct`.

```
pdbstruct = pdbread('nicotinic_receptor.pdb');
```

3 Read only the second model from the `nicotinic_receptor.pdb` file into a MATLAB structure `pdbstruct_Model2`.

```
pdbstruct_Model2 = pdbread('nicotinic_receptor.pdb', 'ModelNum', 2);
```

4 View the atomic coordinate information in the model fields of both MATLAB structures `pdbstruct` and `pdbstruct_Model2`.

```
pdbstruct.Model

ans =

1x4 struct array with fields:
    MDLSerNo
    Atom
    Terminal

pdbstruct_Model2.Model

ans =

    MDLSerNo: 2
```

```
         Atom: [1x1205 struct]
     Terminal: [1x2 struct]
```

5 Read the data from an URL into a MATLAB structure, gfl_pdbstruct.

```
gfl_pdbstruct = pdbread('http://www.rcsb.org/pdb/files/1gfl.pdb');
```

See Also

Bioinformatics Toolbox functions: genpeptread, getpdb, molviewer, pdbdistplot, pdbwrite

Purpose

Write to file using Protein Data Bank (PDB) format

Syntax

```
pdbwrite(File, PDBStruct)
PDBArray = pdbwrite(File, PDBStruct)
```

Arguments

File String specifying either a file name or a path and file name for saving the PDB-formatted data. If you specify only a file name, the file is saved to the MATLAB Current Directory.

> **Tip** After you save the MATLAB structure to a local PDB-formatted file, you can use the `molviewer` function to display and manipulate a 3-D image of the structure.

PDBStruct MATLAB structure containing 3-D protein structure coordinate data, created initially by using the `getpdb` or `pdbread` functions.

> **Note** You can edit this structure to modify its 3-D protein structure data. The coordinate information is stored in the `Model` field of *PDBStruct*.

Return Values

PDBArray Character array in which each row corresponds to a line in a PDB record.

Description

`pdbwrite(`*File*`,` *PDBStruct*`)` writes the contents of the MATLAB structure *PDBStruct* to a PDB-formatted file (ASCII text file) whose path and file name are specified by *File*. In the output file, *File*, the atom serial numbers are preserved. The atomic coordinate records are ordered according to their atom serial numbers.

Tip After you save the MATLAB structure to a local PDB-formatted file, you can use the `molviewer` function to display and manipulate a 3-D image of the structure.

`PDBArray = pdbwrite(File, PDBStruct)` saves the formatted PDB record, converted from the contents of the MATLAB structure *`PDBStruct`*, to *`PDBArray`*, a character array in which each row corresponds to a line in a PDB record.

Note You can edit *`PDBStruct`* to modify its 3-D protein structure data. The coordinate information is stored in the `Model` field of *`PDBStruct`*.

Examples

1. Use the `getpdb` function to retrieve structure information from the Protein Data Bank (PDB) for the green fluorescent protein with identifier `1GFL` , and store the data in the MATLAB structure `gflstruct`.

   ```
   gflstruct = getpdb('1GFL');
   ```

2. Find the *x*-coordinate of the first atom.

   ```
   gflstruct.Model.Atom(1).X

   ans =

     -14.0930
   ```

3. Edit the *x*-coordinate of the first atom.

   ```
   gflstruct.Model.Atom(1).X = -18;
   ```

Note Do not add or remove any `Atom` fields, because the `pdbwrite` function does not allow the number of elements in the structure to change.

---

4 Write the modified MATLAB structure `gflstruct` to a new PDB-formatted file `modified_gfl.pdb` in the `Work` directory on your `C` drive.

```
pdbwrite('c:\work\modified_gfl.pdb', gflstruct);
```

5 Use the `pdbread` function to read the modified PDB file into a MATLAB structure, then confirm that the *x*-coordinate of the first atom has changed.

```
modified_gflstruct = pdbread('c:\work\modified_gfl.pdb')
modified_gflstruct.Model.Atom(1).X

ans =

   -18
```

See Also

Bioinformatics Toolbox functions: `getpdb`, `molviewer`, `pdbread`

pfamhmmread

Purpose Read data from PFAM-HMM file

Syntax

```
Data = pfamhmmread('File')
```

Arguments

File	PFAM-HMM formatted file. Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text of a PFAM-HMM file.

Description

`pfamhmmread` reads data from a PFAM-HMM formatted file (file saved with the function `gethmmprof`) and creates a MATLAB structure.

`Data = pfamhmmread('File')` reads from *File* a Hidden Markov Model described by the PFAM format, and converts it to the MATLAB structure `Data`, containing fields corresponding to annotations and parameters of the model. For more information about the model structure format, see `hmmprofstruct`. *File* can also be a URL or a MATLAB cell array that contains the text of a PFAM formatted file.

`pfamhmmread` is based on the HMMER 2.0 file formats.

Examples

```
pfamhmmread('pf00002.ls')

site='http://www.sanger.ac.uk/';
pfamhmmread([site 'cgi-bin/Pfam/download_hmm.pl?mode=ls&id=7tm_2'])
```

See Also

Bioinformatics Toolbox functions: `gethmmalignment`, `gethmmprof`, `hmmprofalign`, `hmmprofstruct`, `showhmmprof`

Purpose

Create `phytree object`

Syntax

```
Tree = phytree(B)
Tree = phytree(B, D)
Tree = phytree(B, C)
Tree = phytree(BC)
Tree = phytree(..., N)
Tree = phytree
```

Arguments

B	Numeric array of size `[NUMBRANCHES X 2]` in which every row represents a branch of the tree. It contains two pointers to the branch or leaf nodes, which are its children.
C	Column vector with distances for every branch.
D	Column vector with distances from every node to their parent branch.
BC	Combined matrix with pointers to branches or leaves, and distances of branches.
N	Cell array with the names of leaves and branches.

Description

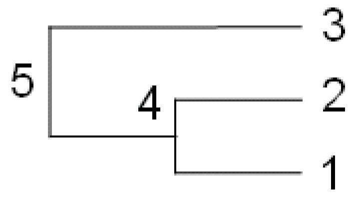
`Tree = phytree(B)` creates an ultrametric phylogenetic tree object. In an ultrametric phylogenetic tree object, all leaves are the same distance from the root.

B is a numeric array of size `[NUMBRANCHES X 2]` in which every row represents a branch of the tree and it contains two pointers to the branch or leaf nodes, which are its children.

Leaf nodes are numbered from `1` to `NUMLEAVES` and branch nodes are numbered from `NUMLEAVES + 1` to `NUMLEAVES + NUMBRANCHES`. Note that because only binary trees are allowed, `NUMLEAVES = NUMBRANCHES + 1`.

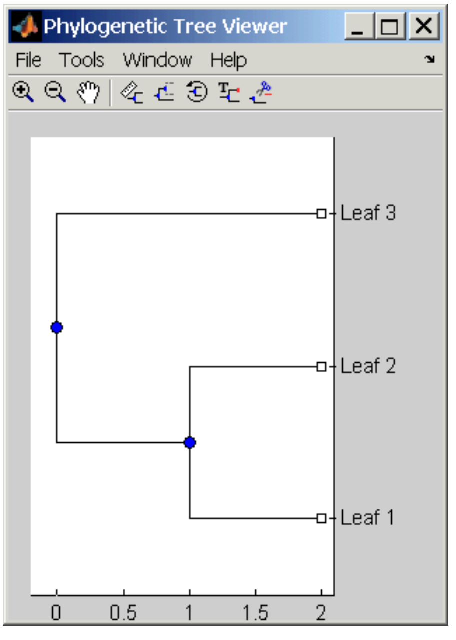
Branches are defined in chronological order (for example, `B(i,:) > NUMLEAVES + i`). As a consequence, the first row can only have pointers to leaves, and the last row must represent the root branch. Parent-child distances are set to 1, unless the child is a leaf and to satisfy the ultrametric condition of the tree its distance is increased.

Given a tree with three leaves and two branches as an example.



In the MATLAB Command Window, type

```
B = [1 2 ; 3 4]
tree = phytree(B)
view(tree)
```



Tree = phytree(*B*, *D*) creates an additive (ultrametric or nonultrametric) phylogenetic tree object with branch distances defined by *D*. *D* is a numeric array of size [NUMNODES X 1] with the distances of every child node (leaf or branch) to its parent branch equal to NUMNODES = NUMLEAVES + NUMBRANCHES. The last distance in *D* is the distance of the root node and is meaningless.

```
b = [1 2 ; 3 4 ]: d = [1 2 1.5 1 0]
view(phytree(b,d)
```

Tree = phytree(*B*, *C*) creates an ultrametric phylogenetic tree object with distances between branches and leaves defined by C. C is a numeric array of size [NUMBRANCHES X 1], which contains the distance from each branch to the leaves. In ultrametric trees, all of the leaves are at the same location (same distance to the root).

```
b = [1 2 ; 3 4]; c = [1 4]'
view(phytree(b,c))
```

Tree = phytree(*BC*) creates an ultrametric phylogenetic binary tree object with branch pointers in BC(:,[1 2]) and branch coordinates in BC(:,3). Same as phytree(B,C).

Tree = phytree(..., *N*) specifies the names for the leaves and/or the branches. *N* is a cell of strings. If NUMEL(N)==NUMLEAVES, then the names are assigned chronologically to the leaves. If NUMEL(N)==NUMBRANCHES, the names are assigned to the branch nodes. If NUMEL(N)==NUMLEAVES + NUMBRANCHES, all the nodes are named. Unassigned names default to 'Leaf #' and/or 'Branch #' as required.

Tree = phytree creates an empty phylogenetic tree object.

Examples

Create a phylogenetic tree for a set of multiply aligned sequences.

```
Sequences = multialignread('aagag.aln')
distances = seqpdist(Sequences)
tree = seqlinkage(distances)
phytreetool(tree)
```

See Also

Bioinformatics Toolbox functions: `phytreeread`, `phytreetool`, `phytreewrite`, `seqlinkage`, `seqneighjoin`, `seqpdist`

Bioinformatics Toolbox object: `phytree object`

Bioinformatics Toolbox methods of phytree object: `get`, `getbyname`, `getcanonical`, `getmatrix`, `getnewickstr`, `pdist`, `plot`, `prune`, `reroot`, `select`, `subtree`, `view`, `weights`

Purpose

Read phylogenetic tree file

Syntax

`Tree = phytreeread(File)`

Arguments

File	Newick-formatted tree files (ASCII text file). Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text for a file.
Tree	`phytree` object created with the function `phytree`.

Description

`Tree = phytreeread(File)` reads a Newick formatted tree file and returns a phytree object in the MATLAB workspace with data from the file.

The NEWICK tree format can be found at

```
http://evolution.genetics.washington.edu/phylip/newicktree.html
```

Note This implementation only allows binary trees. Non-binary trees are translated into a binary tree with extra branches of length 0.

Examples

```
tr = phytreeread('pf00002.tree')
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `gethmmtree`, `phytreetool`, `phytreewrite`

Purpose

View, edit, and explore phylogenetic tree data

Syntax

```
phytreetool(Tree)
phytreetool(File)
```

Arguments

Tree	`Phytree` object created with the functions `phytree` or `phytreeread`.
File	Newick or ClustalW tree formatted file (ASCII text file) with phylogenetic tree data. Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text for a Newick file.

Description

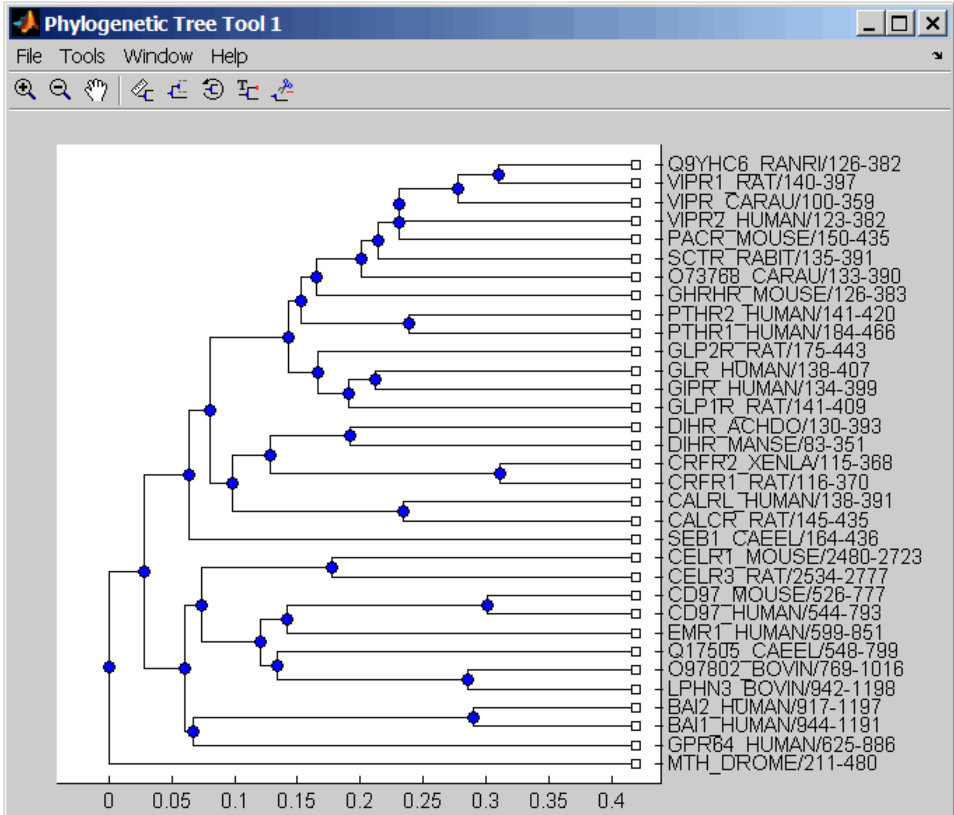
`phytreetool` is an interactive GUI that allows you to view, edit, and explore phylogenetic tree data. This GUI allows branch pruning, reordering, renaming, and distance exploring. It can also open or save Newick formatted files.

`phytreetool(Tree)` loads data from a `phytree` object in the MATLAB workspace into the GUI.

`phytreetool(File)` loads data from a Newick formatted file into the GUI.

Examples

```
tr= phytreeread('pf00002.tree')
phytreetool(tr)
```



See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreeread`, `phytreewrite`

Bioinformatics Toolbox methods of phytree object: `plot`, `view`

phytreewrite

Purpose

Write phylogenetic tree object to Newick-formatted file

Syntax

```
phytreewrite('File', Tree)
phytreewrite(Tree)
```

Arguments

File	Newick-formatted file. Enter either a file name or a path and file name supported by your operating system (ASCII text file).
Tree	Phylogenetic tree object, either created with `phytree` (object constructor function) or imported using the `phytreeread` function.

Description

`phytreewrite('File', Tree)` copies the contents of a `phytree` object from the MATLAB workspace to a file. Data in the file uses the Newick format for describing trees.

The Newick tree format can be found at

```
http://evolution.genetics.washington.edu/phylip/newicktree.html
```

`phytreewrite(Tree)` opens the Save Phylogenetic Tree As dialog box for you to enter or select a file name.

Examples

Read tree data from a Newick-formatted file.

```
tr = phytreeread('pf00002.tree')
```

Remove all the mouse proteins

```
ind = getbyname(tr,'mouse');
tr = prune(tr,ind);
```

```
view(tr)
```

Write pruned tree data to a file.

```
phytreewrite('newtree.tree', tr)
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreeread`, `phytreetool`, `seqlinkage`

Bioinformatics Toolbox object: `phytree object`

Bioinformatics Toolbox methods of phytree object: `getnewickstr`

probelibraryinfo

Purpose

Probe set library information for probe results

Syntax

`ProbeInfo = probelibraryinfo(`*`CELStruct`*`, `*`CDFStruct`*`)`

Description

`ProbeInfo = probelibraryinfo(`*`CELStruct`*`, `*`CDFStruct`*`)`creates a table of information linking the probe data in a CEL file structure with probe set information from a CDF file structure.

`ProbeInfo` is a matrix with three columns and the same number of rows as the probes field of the `CELStruct`. The first column is the probe set ID number to which the probe belongs. (Probes that do not belong to a probe set in the CDF library file have probe set ID equal to `0`.) The second column contains the probe pair number. The third column indicates if the probe is a perfect match (`1`) or mismatch (`-1`) probe.

Note Affymetrix probe pair indexing is `0` based while MATLAB indexing is `1` based. The output from `probelibraryinfo` is `1` based.

Examples

1 Get the file `Drosophila-121502.cel` from

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

2 Read the data into MATLAB.

```
CELStruct = affyread('Drosophila-121502.cel');
CDFStruct = affyread('D:\Affymetrix\LibFiles\...
                     DrosGenome1\DrosGenome1.CDF');
```

3 Extract probe set library information.

```
ProbeInfo = probelibraryinfo(CELStruct, CDFStruct);
```

4 Find out probe set to which the 1104th probe belongs.

```
CDFStruct.ProbeSets(ProbeInfo(1104,1)).Name
```

See Also

Bioinformatics Toolbox functions: `affyread`, `celintensityread`, `probesetlink`, `probesetlookup`, `probesetvalues`

probesetlink

Purpose

Link to NetAffx Web site

Syntax

```
probesetlink(AFFYStruct, ID)
URL = probesetlink(AFFYStruct, ID)
probesetlink(..., 'PropertyName', PropertyValue,...)
probesetlink(..., 'Source', SourceValue),
probesetlink(..., 'Browser', BrowserValue)
probesetlink(..., 'NoDisplay', NoDisplayValue)
```

Description

`probesetlink(`*`AFFYStruct`*`, `*`ID`*`)` displays information from the NetAffx Web site about a probe set (*`ID`*) from the `CHP` or `CDF` structure (*`AFFYStruct`*). *`ID`* can be the index of the probe set or the probe set name.

`URL = probesetlink(`*`AFFYStruct`*`, `*`ID`*`)` returns the URL for the information.

`probesetlink(..., '`*`PropertyName`*`', `*`PropertyValue`*`,...)` defines optional properties using property name/value pairs.

`probesetlink(..., 'Source', `*`SourceValue`*`)`, when *`SourceValue`* is `true`, links to the data source (e.g., GenBank, Flybase) for the probe set.

`probesetlink(..., 'Browser', `*`BrowserValue`*`)`, when *`BrowserValue`* is `true`, displays the information in the system Web browser.

`probesetlink(..., 'NoDisplay', `*`NoDisplayValue`*`)`, when *`NoDisplayValue`* is `true`, returns the URL but does not open a browser.

Note NetAffx Web site requires you to register and provide a user name and password.

Examples

1 Get the file `Drosophila-121502.chp` from

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

2 Read the data into MATLAB.

```
chpStruct = affyread('Drosophila-121502.chp',...
                     'D:\Affymetrix\LibFiles\DrosGenome1')
```

3 Display information from the NetAffx Web site.

```
probesetlink(chpStruct,'AFFX-YEL018w/_at');
```

See Also

Bioinformatics Toolbox functions: `affyread`, `celintensityread`, `probelibraryinfo`, `probesetlookup`, `probesetplot`, `probesetvalues`

probesetlookup

Purpose

Gene name for probe set

Syntax

```
probesetlookup(AFFYStruct, ID)
probesetlookup(AFFYStruct, Name)
[Name, NDX, Description, Source,
   SourceURL] = probesetlookup(...)
```

Description

`probesetlookup(AFFYStruct, ID)` returns the gene name for a probe set `ID` from a `CHP` or `CDF` structure (`AFFYStruct`).

`probesetlookup(AFFYStruct, Name)` returns the probe set ID for a gene name (`Name`) from a `CHP` or `CDF` structure (`AFFYStruct`).

`[Name, NDX, Description, Source, SourceURL] = probesetlookup(...)` returns the name, index into the `CHP` or `CDF` struct, description, source, and source URL and for the probe set.

Note This function requires that you have the GIN file associated with the chip type that you are using in your Affymetrix library directory.

Examples

1 Get the file Drosophila-121502.chp from

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

2 Read the data into MATLAB.

```
chpStruct = affyread('Drosophila-121502.chp',...
                     'D:\Affymetrix\LibFiles\DrosGenome1')
```

3 Get the gene name.

```
probesetlookup(chpStruct,'AFFX-YEL018w/_at')
```

See Also

Bioinformatics Toolbox functions: `affyread`, `celintensityread`, `probelibraryinfo`, `probesetlink`, `probesetplot`, `probesetvalues`, `rmabackadj`

Purpose

Plot values for Affymetrix CHP file probe set

Syntax

```
probesetplot(CHPStruct, ID, 'PropertyName', PropertyValue)
probesetplot(..., 'GeneName', GeneNameValue)
probesetplot(..., 'Field', FieldValue)
probesetplot(..., 'ShowStats',ShowStatsValue)
```

Description

`probesetplot(CHPStruct, ID, 'PropertyName', PropertyValue)` plots the PM and MM intensity values for probe set `ID`. `CHPStruct` is a structure created from an Affymetrix `CHP` file. `ID` can be the index of the probe set or the probe set name. Note: the probe set numbers for a `CHP` file use `0` based indexing while MATLAB uses `1` based indexing. `CHPStruct.ProbeSets(1)` has ProbeSetNumber `0`.

`probesetplot(..., 'GeneName', GeneNameValue)` when `GeneName` is `true`, uses the gene name, rather than the probeset name for the title.

`probesetplot(..., 'Field', FieldValue)` shows the data for a field (`FieldValue`). Valid fieldnames are: `Background`, `Intensity`, `StdDev`, `Pixels`, and `Outlier`.

`probesetplot(..., 'ShowStats',ShowStatsValue)` when `ShowStats` is `true`, adds mean and standard deviation lines to the plot.

Examples

1 Get the file Drosophila-121502.chp from

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

2 Read the data into MATLAB.

```
chpStruct = affyread('Drosophila-121502.chp',...
                     'D:\Affymetrix\LibFiles\DrosGenome1')
```

3 Plots PM and MM intensity values.

```
probesetplot(chpStruct,'AFFX-YEL018w/_at','showstats',true);
```

See Also

Bioinformatics Toolbox functions: `affyread`, `celintensityread`, `probesetlink`, `probesetlookup`

probesetvalues

Purpose

Probe set values from probe results

Syntax

```
PSValues = probesetvalues(CELStruct,CDFStruct,PS)
```

Description

PSValues = probesetvalues(*CELStruct*,*CDFStruct*,*PS*) creates a table of values for a probe set (*PS*) from the probe data in a CEL file structure (*CELStruct*). *PS* is a probe set index or probe set name from the CDF library file structure (*CDFStruct*). *PSValues* is a matrix with 18 columns and one row for each probe pair in the probe set. The columns correspond to the fields in a CHP probe set data structure:

```
'ProbeSetNumber'
     'ProbePairNumber'
     'UseProbePair'
     'Background'
     'PMPosX'
     'PMPosY'
     'PMIntensity'
     'PMStdDev'
     'PMPixels'
     'PMOutlier'
     'PMMasked'
     'MMPosX'
     'MMPosY'
     'MMIntensity'
     'MMStdDev'
     'MMPixels'
     'MMOutlier'
     'MMMasked'
```

There are some minor differences between the output of this function and the data in a CHP file. The PM and MM Intensity values in the CHP file are normalized by the Affymetrix software. This function returns the raw intensity values. The 'UseProbePair' and 'Background' fields are only returned by this function for compatibility with the CHP probe set data structure and are always set to zero.

Examples

1 Get the file `Drosophila-121502.cel` from

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

2 Read the data into MATLAB.

```
celStruct = affyread('Drosophila-121502.cel');
cdfStruct = affyread('D:\Affymetrix\LibFiles\DrosGenome1\...
                     DrosGenome1.CDF');
```

3 Get the values for probe set 147439_at.

```
psvals = probesetvalues(celStruct,cdfStruct,'147439_at')
```

See Also

Bioinformatics Toolbox functions: `affyread`, `celintensityread`, `probelibraryinfo`, `probesetlink`, `probesetlookup`, `rmabackadj`

profalign

Purpose

Align two profiles using Needleman-Wunsch global alignment

Syntax

```
Prof = profalign(Prof1, Prof2)
[Prof, H1, H2] = profalign(Prof1, Prof2)
profalign(..., 'PropertyName', PropertyValue,...)
profalign(..., 'ScoringMatrix', ScoringMatrixValue)
profalign(..., 'GapOpen', {G1Value, G2Value})
profalign(..., 'ExtendGap', {E1Value, E2Value})
profalign(..., 'ExistingGapAdjust', ExistingGapAdjustValue)
profalign(..., 'TerminalGapAdjust', TerminalGapAdjustValue)
profalign(..., 'ShowScore', ShowScoreValue)
```

Description

`Prof = profalign(Prof1, Prof2)` returns a new profile (`Prof`) for the optimal global alignment of two profiles (`Prof1`, `Prof2`). The profiles (`Prof1`, `Prof2`) are numeric arrays of size `[(4 or 5 or 20 or 21) x Profile Length]` with counts or weighted profiles. Weighted profiles are used to down-weight similar sequences and up-weight divergent sequences. The output profile is a numeric matrix of size `[(5 or 21) x New Profile Length]` where the last row represents gaps. Original gaps in the input profiles are preserved. The output profile is the result of adding the aligned columns of the input profiles.

`[Prof, H1, H2] = profalign(Prof1, Prof2)` returns pointers that indicate how to rearrange the columns of the original profiles into the new profile.

`profalign(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`profalign(..., 'ScoringMatrix', ScoringMatrixValue)` defines the scoring matrix (`ScoringMatrixValue`) to be used for the alignment. The default is `'BLOSUM50'` for amino acids or `'NUC44'` for nucleotide sequences.

`profalign(..., 'GapOpen', {G1Value, G2Value})` sets the penalties for opening a gap in the first and second profiles respectively. `G1Value` and `G2Value` can be either scalars or vectors. When using a vector, the number of elements is one more than the length of the input profile. Every element indicates the position specific penalty for opening a gap between two consecutive symbols in the sequence. The first and the last elements are the gap penalties used at the ends of the sequence. The default gap open penalties are {10,10}.

profalign(..., 'ExtendGap', {*E1Value*, *E2Value*}) sets the penalties for extending a gap in the first and second profile respectively. *E1Value* and *E2Value* can be either scalars or vectors. When using a vector, the number of elements is one more than the length of the input profile. Every element indicates the position specific penalty for extending a gap between two consecutive symbols in the sequence. The first and the last elements are the gap penalties used at the ends of the sequence. If ExtendGap is not specified, then extensions to gaps are scored with the same value as GapOpen.

profalign(..., 'ExistingGapAdjust', *ExistingGapAdjustValue*), if *ExistingGapAdjustValue* is false, turns off the automatic adjustment based on existing gaps of the position-specific penalties for opening a gap. When *ExistingGapAdjustValue* is true, for every profile position, profalign proportionally lowers the penalty for opening a gap toward the penalty of extending a gap based on the proportion of gaps found in the contiguous symbols and on the weight of the input profile.

profalign(..., 'TerminalGapAdjust', *TerminalGapAdjustValue*), when *TerminalGapAdjustValue* is true, adjusts the penalty for opening a gap at the ends of the sequence to be equal to the penalty for extending a gap. Default is false.

profalign(..., 'ShowScore', *ShowScoreValue*), when *ShowScoreValue* is true, displays the scoring space and the winning path.

Examples

1 Read in sequences and create profiles.

```
ma1 = ['RGTANCDMQDA';'RGTAHCDMQDA';'RRRAPCDL-DA'];
ma2 = ['RGTHCDLADAT';'RGTACDMADAA'];
p1  = seqprofile(ma1,'gaps','all','counts',true);
p2  = seqprofile(ma2,'counts',true);
```

2 Merge two profiles into a single one by aligning them.

```
p = profalign(p1,p2);
seqlogo(p)
```

3 Use the output pointers to generate the multiple alignment.

```
[p, h1, h2] = profalign(p1,p2);
ma = repmat('-',5,12);
ma(1:3,h1) = ma1;
ma(4:5,h2) = ma2;
disp(ma)
```

4 Increase the gap penalty before cysteine in the second profile.

```
gapVec = 10 + [p2(aa2int('C'),:) 0] * 10
p3 = profalign(p1,p2,'gapopen',{10,gapVec});
seqlogo(p3)
```

5 Add a new sequence to a profile without inserting new gaps into the profile.

```
gapVec = [0 inf(1,11) 0];
p4 = profalign(p3,seqprofile('PLHFMSVLWDVQQWP'),...
               gapopen',{gapVec,10});
seqlogo(p4)
```

See Also

Bioinformatics Toolbox functions `hmmprofalign`, `multialign`, `nwalign`, `seqprofile`, `seqconsensus`

Purpose

Characteristics for amino acid sequences

Syntax

```
proteinplot (SeqAA)
```

Arguments

SeqAA	Amino acid sequence or a structure with a field `Sequence` containing an amino acid sequence.

Description

`proteinplot (SeqAA)` loads an amino acid sequence into the protein plot GUI. `proteinplot` is a tool for analyzing a single amino acid sequence. You can use the results from `proteinplot` to compare the properties of several amino acid sequences. It displays smoothed line plots of various properties such as the hydrophobicity of the amino acids in the sequence.

Importing Sequences into proteinplot

1. In the MATLAB Command Window, type

   ```
   proteinplot(Seq_AA)
   ```

   The `proteinplot` interface opens and the sequence `Seq_AA` is shown in the **Sequence** text box.

2. Alternatively, type or paste an amino acid sequence into the **Sequence** text box.

You can import a sequence with the Import dialog box:

1. Click the **Import Sequence** button. The Import dialog box opens.

2. From the **Import From** list, select a variable in the MATLAB workspace, ASCII text file, FASTA formatted file, GenPept formatted file, or accession number in the GenPept database.

Information About the Properties

You can also access information about the properties from the **Help** menu.

1. From the **Help** menu, click **References**. The Help Browser opens with a list of properties and references.

2. Scroll down to locate the property you are interested in studying.

Working with Properties

When you click on a property a smoothed plot of the property values along the sequence will be displayed. Multiple properties can be selected from the list by holding down Shift or Ctrl while selecting properties. When two properties are selected, the plots are displayed using a PLOTYY-style layout, with one *y*-axis on the left and one on the right. For all other selections, a single *y*-axis is displayed. When displaying one or two properties, the *y* values displayed are the actual property values. When three or more properties are displayed, the values are normalized to the range 0-1.

You can add your own property values by clicking on the Add button next to the property list. This will open up a dialog that allows you to specify the values for each of the amino acids. The Display Text box allows you to specify the text that will be displayed in the selection box on the main `proteinplot` window. You can also save the property values to an m-file for future use by typing a file name into the Filename box.

The Terminal Selection boxes allow you to choose to plot only part of the sequence. By default all of the sequence is plotted. The default smoothing method is an unweighted linear moving average with a window length of five residues. You can change this using the "Configuration Values" dialog from the Edit menu. The dialog allows you to select the window length from `5` to `29` residues. You can modify the shape of the smoothing window by changing the edge weighting factor. And you can choose the smoothing function to be a linear moving average, an exponential moving average or a linear Lowess smoothing.

The File menu allows you to Import a sequence, save the plot that you have created to a `FIG` file, you can export the data values in the figure to a workspace variable or to a MAT file, you can export the figure to a normal figure window for customizing, and you can print the figure.

The Edit menu allows you to create a new property, to reset the property values to the default values, and to modify the smoothing parameters with the Configuration Values menu item.

The View menu allows you to turn the toolbar on and off, and to add a legend to the plot.

The Tools menu allows you to zoom in and zoom out of the plot, to view Data Statistics such as mean, minimum and maximum values of the plot, and to normalize the values of the plot from `0` to `1`.

The Help menu allows you to view this document and to see the references for the sequence properties built into `proteinplot`

See Also

Bioinformatics Toolbox functions: `aacount`, `atomiccomp`, `molviewer`, `molweight`, `pdbdistplot`, `seqtool`

MATLAB function: `plotyy`

proteinpropplot

Purpose Plot properties of amino acid sequence

Syntax

```
proteinpropplot (SeqAA)
proteinpropplot(SeqAA, ...'PropertyTitle',
PropertyTitleValue, ...)
proteinpropplot(SeqAA, ...'Startat', StartatValue, ...)
proteinpropplot(SeqAA, ...'Endat', EndatValue, ...)
proteinpropplot(SeqAA, ...'Smoothing', SmoothingValue, ...)
proteinpropplot(SeqAA, ...'EdgeWeight',
EdgeWeightValue, ...)
proteinpropplot(SeqAA, ...'WindowLength',
WindowLengthValue,
    ...)
```

Arguments

SeqAA

Amino acid sequence. Enter any of the following:

- Character string of letters representing an amino acid
- Vector of integers representing an amino acid, such as returned by `aa2int`
- Structure containing a `Sequence` field that contains an amino acid sequence, such as returned by `getembl`, `getgenpept`, or `getpdb`

PropertyTitleValue

String that specifies the property to plot. Default is `Hydrophobicity (Kyte & Doolittle)`. To display a list of properties to plot, enter a empty string for *PropertyTitleValue*. For example, type:

```
proteinpropplot(sequence, 'propertytitle', '')
```

Tip To access references for the properties, view the `proteinpropplot` m-file.

StartatValue

Integer that specifies the starting point for the plot from the N-terminal end of the amino acid sequence *SeqAA*. Default is `1`.

EndatValue

Integer that specifies the ending point for the plot from the N-terminal end of the amino acid sequence *SeqAA*. Default is `length(`*SeqAA*`)`.

SmoothingValue

String the specifies the smoothing method. Choices are:

- `linear` (default)
- `exponential`
- `lowess`

EdgeWeightValue	Value that specifies the edge weight used for linear and exponential smoothing methods. Decreasing this value emphasizes peaks in the plot. Choices are any value ≥0 and ≤1. Default is 1.
WindowLengthValue	Integer that specifies the window length for the smoothing method. Increasing this value gives a smoother plot that shows less detail. Default is 11.

Description

`proteinpropplot (`*`SeqAA`*`)` displays a plot of the hydrophobicity (Kyte and Doolittle, 1982) of the residues in sequence `SeqAA`.

`proteinpropplot(`*`SeqAA`*`, ...'`*`PropertyName`*`',` *`PropertyValue`*`, ...)` calls `proteinpropplot` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`proteinpropplot(`*`SeqAA`*`, ...'PropertyTitle',` *`PropertyTitleValue`*`, ...)` specifies a property to plot for the amino acid sequence *`SeqAA`*. Default is `Hydrophobicity (Kyte & Doolittle)`. To display a list of possible properties to plot, enter an empty string for *`PropertyTitleValue`*. For example, type:

```
proteinpropplot(sequence, 'propertytitle', '')
```

Tip To access references for the properties, view the `proteinpropplot` m-file.

`proteinpropplot(`*`SeqAA`*`, ...'Startat',` *`StartatValue`*`, ...)` specifies the starting point for the plot from the N-terminal end of the amino acid sequence *`SeqAA`*. Default is `1`.

`proteinpropplot(`*`SeqAA`*`, ...'Endat', `*`EndatValue`*`, ...)` specifies the ending point for the plot from the N-terminal end of the amino acid sequence *SeqAA*. Default is `length(`*`SeqAA`*`)`.

`proteinpropplot(`*`SeqAA`*`, ...'Smoothing', `*`SmoothingValue`*`, ...)` specifies the smoothing method. Choices are:

- `linear` (default)
- `exponential`
- `lowess`

`proteinpropplot(`*`SeqAA`*`, ...'EdgeWeight',` *`EdgeWeightValue`*`, ...)` specifies the edge weight used for linear and exponential smoothing methods. Decreasing this value emphasizes peaks in the plot. Choices are any value ≥`0` and ≤`1`. Default is `1`.

`proteinpropplot(`*`SeqAA`*`, ...'WindowLength',` *`WindowLengthValue`*`, ...)` specifies the window length for the smoothing method. Increasing this value gives a smoother plot that shows less detail. Default is `11`.

Examples

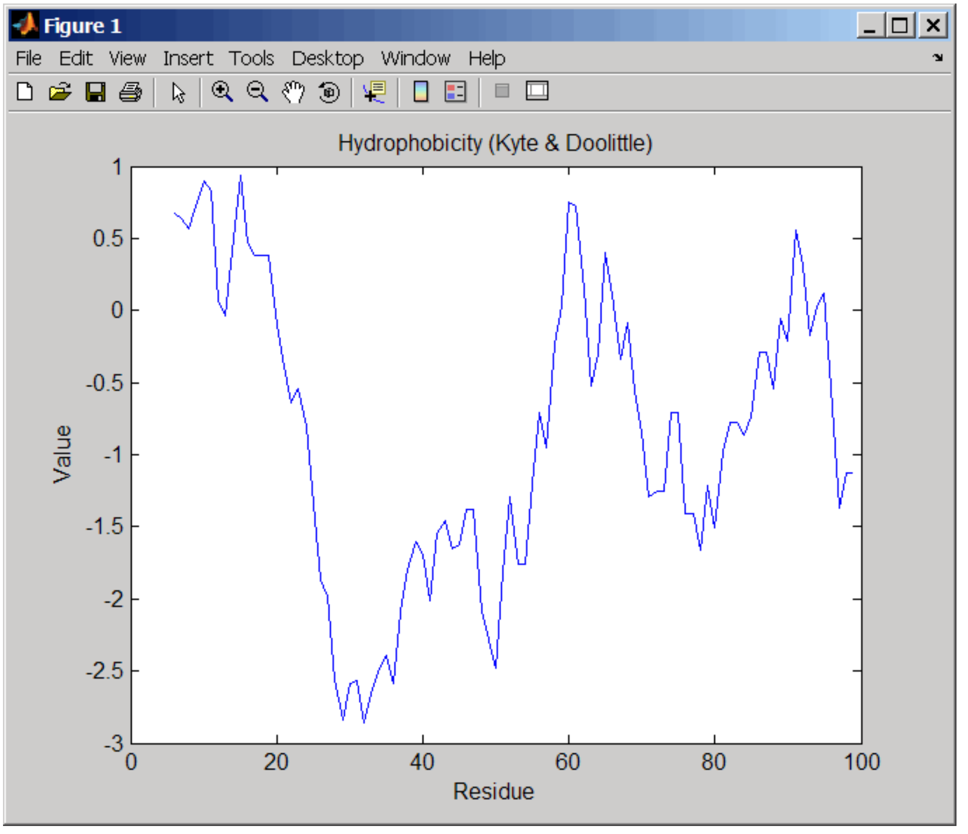
Plotting Hydrophobicity

1 Use the `getpdb` function to retrieve a protein sequence.

```
prion = getpdb('1HJM', 'SEQUENCEONLY', true);
```

2 Plot the hydrophobicity (Kyte and Doolittle, 1982) of the residues in the sequence.

```
proteinpropplot(prion)
```



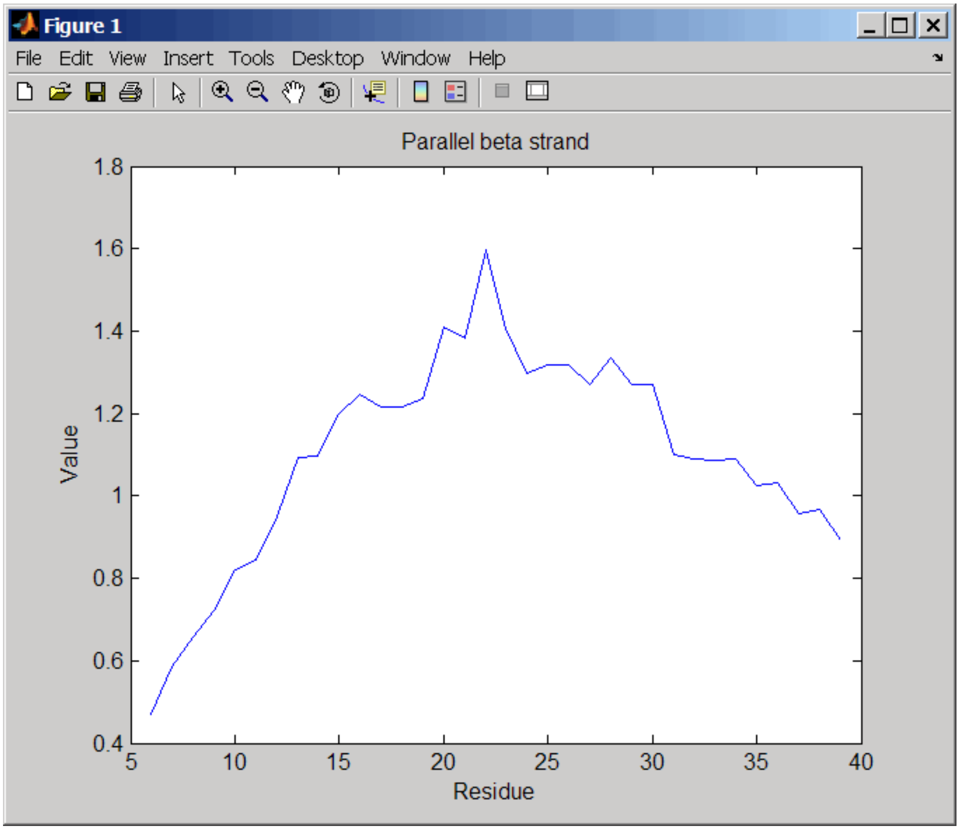
Plotting Parallel Beta Strand

1 Use the `getgenpept` function to retrieve a protein sequence.

```
s = getgenpept('aad50640');
```

2 Plot the conformational preference for parallel beta strand for the residues in the sequence.

```
proteinpropplot(s,'propertytitle','Parallel beta strand')
```



References

[1] Kyte, J., and Doolittle, R.F. (1982). A simple method for displaying the hydropathic character of a protein. J Mol Biol *157(1)*, 105–132.

See Also

Bioinformatics Toolbox functions: `aacount`, `atomiccomp`, `molviewer`, `molweight`, `pdbdistplot`, `proteinplot`, `ramachandran`, `seqtool`

MATLAB function: `plotyy`

quantilenorm

Purpose

Quantile normalization over multiple arrays

Syntax

```
NormData = quantilenorm(Data)
NormData = quantilenorm(...,'MEDIAN', true)
NormData = quantilenorm(...,'DISPLAY', true)
```

Description

`NormData = quantilenorm(Data)`, where the columns of `Data` correspond to separate chips, normalizes the distributions of the values in each column.

Note If `Data` contains NaN values, then `NormData` will also contain NaN values at the corresponding positions.

`NormData = quantilenorm(...,'MEDIAN', true)` takes the median of the ranked values instead of the mean.

`NormData = quantilenorm(...,'DISPLAY', true)` plots the distributions of the columns and of the normalized data.

Examples

```
load yeastdata
normYeastValues = quantilenorm(yeastvalues,'display',1);
```

See Also

`malowess`, `manorm`, `rmabackadj`, `rmasummary`

Purpose

Draw Ramachandran plot for Protein Data Bank (PDB) data

Syntax

```
ramachandran('PDBid')
ramachandran('File')
ramachandran(PDBData)
Angles = ramachandran(...)
[Angles, Handle] = ramachandran(...)
```

Arguments

PDBid	Unique identifier for a protein structure record. Each structure in the PDB is represented by a 4-character alphanumeric identifier. For example, `4hhb` is the identification code for hemoglobin.
File	Protein Data Bank (PDB) formatted file (ASCII text file). Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text for a PDB file.
PDBData	MATLAB structure with PDB formatted data.

Description

`ramachandran` generates a plot of the torsion angle PHI (torsion angle between the `'C-N-CA-C'` atoms) and the torsion angle PSI (torsion angle between the `'N-CA-C-N'` atoms) of the protein sequence.

`ramachandran('`*PDBid*`')` generates the Ramachandran plot for the protein with PDB code `ID`.

`ramachandran('`*File*`')` generates the Ramachandran plot for protein stored in the PDB file *File*.

`ramachandran(PDBData)` generates the Ramachandran plot for the protein stored in the structure `PDBData`, where `PDBData` is a MATLAB structure obtained by using `pdbread` or `getpdb`.

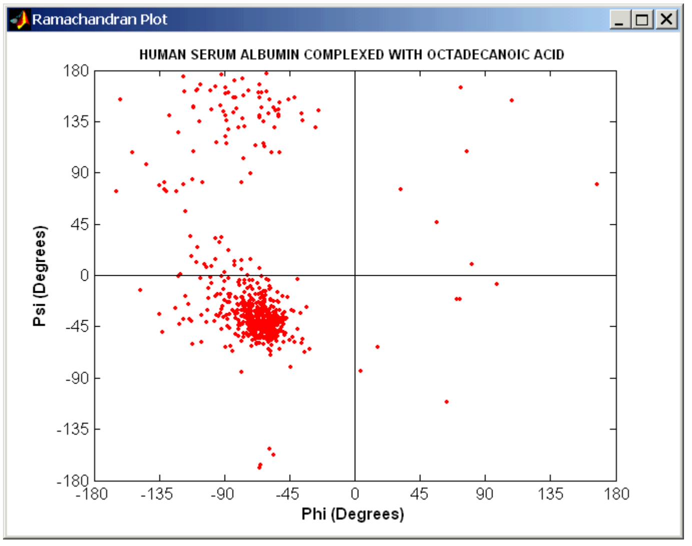
`Angles = ramachandran(...)` returns an array of the torsion angles PHI, PSI, and OMEGA for the residue sequence.

`[Angles, Handle] = ramachandran(...)` returns a handle to the plot.

Examples

Generate the Ramachandran plot for the human serum albumin complexed with octadecanoic acid.

```
ramachandran('1E7I')
```



See Also

Bioinformatics Toolbox functions: `getpdb`,`molviewer`, `pdbdistplot`, `pdbread`

Purpose

Generate randomized subset of features

Syntax

```
[IDX, Z] = randfeatures(X, Group, 'PropertyName',
   PropertyValue...)
randfeatures(..., 'Classifier', C)
randfeatures(..., 'ClassOptions', CO)
randfeatures(..., 'PerformanceThreshold', PT)
randfeatures(..., 'ConfidenceThreshold', CT)
randfeatures(..., 'SubsetSize', SS)
randfeatures(..., 'PoolSize', PS)
randfeatures(..., 'NumberOfIndices', N)
randfeatures(..., 'CrossNorm', CN)
randfeatures(..., 'Verbose', VerboseValue)
```

Description

`[IDX, Z] = randfeatures(X, Group, '`*`PropertyName`*`',` *`PropertyValue`*`...)` performs a randomized subset feature search reinforced by classification. `randfeatures` randomly generates subsets of features used to classify the samples. Every subset is evaluated with the apparent error. Only the best subsets are kept, and they are joined into a single final pool. The cardinality for every feature in the pool gives the measurement of the significance.

`X` contains the training samples. Every column of `X` is an observed vector. `Group` contains the class labels. `Group` can be a numeric vector or a cell array of strings; `numel(Group)` must be the same as the number of columns in `X`, and `numel(unique(Group))` must be greater than or equal to `2`. `Z` is the classification significance for every feature. `IDX` contains the indices after sorting `Z`; i.e., the first one points to the most significant feature.

`randfeatures(..., 'Classifier', C)` sets the classifier. Options are

```
'da'   (default)  Discriminant analysis
'knn'             K nearest neighbors
```

`randfeatures(..., 'ClassOptions', CO)`is a cell with extra options for the selected classifier. Defaults are

{5,'correlation','consensus'} for KNN and {'linear'} for DA. See knnclassify and classify for more information.

randfeatures(..., 'PerformanceThreshold', PT) sets the correct classification threshold used to pick the subsets included in the final pool. Default is 0.8 (80%).

randfeatures(..., 'ConfidenceThreshold', CT) uses the posterior probability of the discriminant analysis to invalidate classified subvectors with low confidence. This option is only valid when Classifier is 'da'. Using it has the same effect as using 'consensus' in KNN; i.e., it makes the selection of approved subsets very stringent. Default is 0.95.^(number of classes).

randfeatures(..., 'SubsetSize', SS) sets the number of features considered in every subset. Default is 20.

randfeatures(..., 'PoolSize', PS) sets the targeted number of accepted subsets for the final pool. Default is 1000.

randfeatures(..., 'NumberOfIndices', N) sets the number of output indices in IDX. Default is the same as the number of features.

randfeatures(..., 'CrossNorm', CN) applies independent normalization across the observations for every feature. Cross-normalization ensures comparability among different features, although it is not always necessary because the selected classifier properties might already account for this. Options are

```
'none' (default)  Intensities are not cross-normalized.
'meanvar'         x_new = (x - mean(x))/std(x)
'softmax'         x_new = (1+exp((mean(x)-x)/std(x)))^-1
'minmax'          x_new = (x - min(x))/(max(x)-min(x))
```

randfeatures(..., 'Verbose', VerboseValue), when Verbose is true, turns off verbosity. Default is true.

Examples

Find a reduced set of genes that is sufficient for classification of all the cancer types in the t-matrix NCI60 data set. Load sample data.

```
load NCI60tmatrix
```

Select features.

```
I = randfeatures(X,GROUP,'SubsetSize',15,'Classifier','da');
```

Test features with a linear discriminant classifier.

```
C = classify(X(I(1:25),:)',X(I(1:25),:)',GROUP);
cp = classperf(GROUP,C);
cp.CorrectRate
```

See Also

Bioinformatics Toolbox functions: `classperf`, `crossvalind`, `knnclassify`, `rankfeatures`, `svmclassify`

Statistics Toolbox function: `classify`

randseq

Purpose

Generate random sequence from finite alphabet

Syntax

```
Seq = randseq(SeqLength)
Seq = randseq(SeqLength, ...'Alphabet', AlphabetValue, ...)
Seq = randseq(SeqLength, ...'Weights', WeightsValue, ...)
Seq = randseq(SeqLength, ...'FromStructure',
    FromStructureValue, ...)
Seq = randseq(SeqLength, ...'Case', CaseValue, ...)
Seq = randseq(SeqLength, ...'DataType', DataTypeValue, ...)
```

Arguments

SeqLength	Number of amino acids or nucleotides in random sequence .
AlphabetValue	Property to select the alphabet for the sequence. Enter `'dna'`(default), `'rna'`, or `'amino'`.
WeightsValue	Property to specify a weighted random sequence.
FromStructureValue	Property to specify a weighted random sequence using output structures from the functions from `basecount`, `dimercount`, `codoncount`, or `aacount`.
CaseValue	Property to select the case of letters in a sequence when`Alphabet` is `'char'`. Values are`'upper'` (default) or `'lower'`.
DataTypeValue	Property to select the data type for a sequence. Values are `'char'`(default) for letter sequences, and `'uint8'` or `'double'` for numeric sequences. Creates a sequence as an array of *`DataType`*.

Description

`Seq` `= randseq(`*`SeqLength`*`)` creates a random sequence with a length specified by *`SeqLength`*.

`Seq = randseq(SeqLength, ...'PropertyName', PropertyValue, ...)` calls `randseq` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`Seq = randseq(SeqLength, ...'Alphabet', AlphabetValue, ...)` generates a sequence from a specific alphabet.

`Seq = randseq(SeqLength, ...'Weights', WeightsValue, ...)` creates a weighted random sequence where the `i`th letter of the sequence alphabet is selected with weight `W(i)`. The weight vector is usually a probability vector or a frequency count vector. Note that the `i`th element of the nucleotide alphabet is given by `int2nt(i)`, and the `i`th element of the amino acid alphabet is given by `int2aa(i)`.

`Seq = randseq(SeqLength, ...'FromStructure', FromStructureValue, ...)` creates a weighted random sequence with weights given by the output structure from `basecount`, `dimercount`, `codoncount`, or `aacount`.

`Seq = randseq(SeqLength, ...'Case', CaseValue, ...)` specifies the case for a letter sequence.

`Seq = randseq(SeqLength, ...'DataType', DataTypeValue, ...)` specifies the data type for the sequence array.

Examples

Generate a random DNA sequence.

```
randseq(20)

ans =
TAGCTGGCCAAGCGAGCTTG
```

Generate a random RNA sequence.

```
randseq(20,'alphabet','rna')

ans =
```

```
GCUGCGGCGGUUGUAUCCUG
```

Generate a random protein sequence.

```
randseq(20,'alphabet','amino')

ans =
DYKMCLYEFGMFGHFTGHKK
```

See Also

Statistics Toolbox functions: `hmmgenerate`, `randsample`

MATLAB functions: `rand`, `randperm`

Purpose

Rank key features by class separability criteria

Syntax

```
[IDX, Z] = rankfeatures(X, Group)
[IDX, Z] = rankfeatures(X, Group, ...'Criterion',
CriterionValue, ...)
[IDX, Z] = rankfeatures(X, Group, ...'CCWeighting', ALPHA,
   ...)
[IDX, Z] = rankfeatures(X, Group, ...'NWeighting',
BETA, ...)
[IDX, Z] = rankfeatures(X, Group, ...'NumberOfIndices', N,
   ...)
[IDX, Z] = rankfeatures(X, Group, ...'CrossNorm', CN, ...)
```

Description

`[IDX, Z] = rankfeatures(X, Group)` ranks the features in *X* using an independent evaluation criterion for binary classification. *X* is a matrix where every column is an observed vector and the number of rows corresponds to the original number of features. *Group* contains the class labels.

IDX is the list of indices to the rows in *X* with the most significant features. *Z* is the absolute value of the criterion used (see below).

Group can be a numeric vector or a cell array of strings; `numel(Group)` is the same as the number of columns in *X*, and `numel(unique(Group))` is equal to `2`.

`[IDX, Z] = rankfeatures(X, Group, ...'PropertyName', PropertyValue, ...)` calls `rankfeatures` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows.

`[IDX, Z] = rankfeatures(X, Group, ...'Criterion', CriterionValue, ...)` sets the criterion used to assess the significance of every feature for separating two labeled groups. Choices are:

`'ttest'` (default)	Absolute value two-sample t-test with pooled variance estimate
`'entropy'`	Relative entropy, also known as Kullback-Lieber distance or divergence
`'brattacharyya'`	Minimum attainable classification error or Chernoff bound
`'roc'`	Area between the empirical receiver operating characteristic (ROC) curve and the random classifier slope
`'wilcoxon'`	Absolute value of the u-statistic of a two-sample unpaired Wilcoxon test, also known as Mann-Whitney

Note `'ttest'`, `'entropy'`, and `'brattacharyya'` assume normal distributed classes while `'roc'` and `'wilcoxon'` are nonparametric tests. All tests are feature independent.

`[IDX, Z] = rankfeatures(X, Group, ...'CCWeighting', ALPHA, ...)` uses correlation information to outweigh the `Z` value of potential features using `Z * (1-ALPHA*(RHO))` where `RHO` is the average of the absolute values of the cross-correlation coefficient between the candidate feature and all previously selected features. `ALPHA` sets the weighting factor. It is a scalar value between `0` and `1`. When `ALPHA` is `0` (default) potential features are not weighted. A large value of `RHO` (close to `1`) outweighs the significance statistic; this means that features that are highly correlated with the features already picked are less likely to be included in the output list.

`[IDX, Z] = rankfeatures(X, Group, ...'NWeighting', BETA, ...)` uses regional information to outweigh the `Z` value of potential features using `Z * (1-exp(-(DIST/BETA).^2))` where `DIST` is the distance (in rows) between the candidate feature and previously selected features. `BETA` sets the weighting factor. It is greater than or equal to `0`. When `BETA` is `0` (default) potential features are not weighted.

A small `DIST` (close to `0`) outweighs the significance statistics of only close features. This means that features that are close to already picked features are less likely to be included in the output list. This option is useful for extracting features from time series with temporal correlation.

`BETA` can also be a function of the feature location, specified using `@` or an anonymous function. In both cases `rankfeatures` passes the row position of the feature to `BETA()` and expects back a value greater than or equal to `0`.

Note You can use `'CCWeighting'` and `'NWeighting'` together.

`[IDX, Z] = rankfeatures(X, Group, ...'NumberOfIndices', N, ...)` sets the number of output indices in *`IDX`*. Default is the same as the number of features when *`ALPHA`* and *`BETA`* are `0`, or `20` otherwise.

`[IDX, Z] = rankfeatures(X, Group, ...'CrossNorm', CN, ...)` applies independent normalization across the observations for every feature. Cross-normalization ensures comparability among different features, although it is not always necessary because the selected criterion might already account for this. Choices are:

`'none'` (default)	Intensities are not cross-normalized.
`'meanvar'`	`x_new = (x - mean(x))/std(x)`
`'softmax'`	`x_new = (1+exp((mean(x)-x)/std(x)))^-1`
`'minmax'`	`x_new = (x - min(x))/(max(x)-min(x))`

Examples

1 Find a reduced set of genes that is sufficient for differentiating breast cancer cells from all other types of cancer in the t-matrix NCI60 data set. Load sample data.

```
load NCI60tmatrix
```

2 Get a logical index vector to the breast cancer cells.

```
BC = GROUP == 8;
```

3 Select features.

```
I = rankfeatures(X,BC,'NumberOfIndices',12);
```

4 Test features with a linear discriminant classifier.

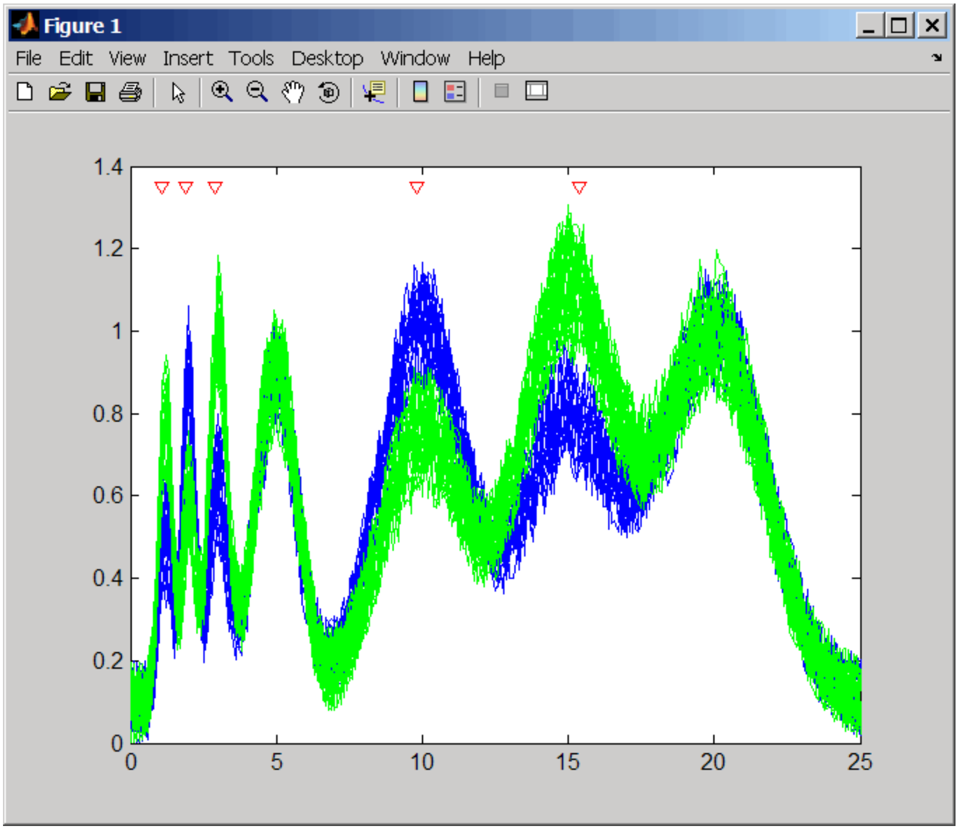
```
C = classify(X(I,:)',X(I,:)',double(BC));
cp = classperf(BC,C);
cp.CorrectRate

ans =

     1
```

5 Use cross-correlation weighting to further reduce the required number of genes.

```
I = rankfeatures(X,BC,'CCWeighting',0.7,'NumberOfIndices',8);
C = classify(X(I,:)',X(I,:)',double(BC));
cp = classperf(BC,C);
cp.CorrectRate

ans =

     1
```

6 Find the discriminant peaks of two groups of signals with Gaussian pulses modulated by two different sources.

```
load GaussianPulses
f = rankfeatures(y',grp,'NWeighting',@(x) x/10+5,'NumberOfIndices',5);
plot(t,y(grp==1,:),'b',t,y(grp==2,:),'g',t(f),1.35,'vr')
```



See Also

Bioinformatics Toolbox functions: `classperf`, `crossvalind`, `randfeatures`, `svmclassify`

Statistics Toolbox function: `classify`

rebasecuts

Purpose

Find restriction enzymes that cut protein sequence

Syntax

```
[Enzymes, Sites] = rebasecuts(SeqNT)
rebasecuts(SeqNT, Group)
rebasecuts(SeqNT, [Q, R])
rebasecuts(SeqNT, S)
```

Arguments

SeqNT	Nucleotide sequence.
Enzymes	Cell array with the names of restriction enzymes from REBASE Version 412.
Sites	Vector of cut sites with the base number before every cut relative to the sequence.
Group	Cell array with the names of valid restriction enzymes.
Q, *R*, *S*	Base positions.

Description

`[Enzymes, Sites] = rebasecuts(SeqNT)` finds all the restriction enzymes that cut a nucleotide sequence (*SeqNT*).

`rebasecuts(SeqNT, Group)` limits the search to a specified list of enzymes (*Group*).

`rebasecuts(SeqNT, [Q, R])` limits the search to those enzymes that cut after a specified base position (*Q*) and before a specified base position (*R*) relative to the sequence.

`rebasecuts(SeqNT, S)` limits the search to those enzymes that cut just after a specified base position (*S*).

REBASE, the Restriction Enzyme Database, is a collection of information about restriction enzymes and related proteins. For more information about REBASE, see

```
http://rebase.neb.com/rebase/rebase.html
```

Example

1 Enter a nucleotide sequence.

```
seq = 'AGAGGGGTACGCGCTCTGAAAAGCGGGAACCTCGTGGCGCTTTATTAA'
```

2 Look for all possible cleavage sites in the sequence seq.

```
[enzymes sites] = rebasecuts(seq)
```

3 Find where restriction enzymes CfoI and Tru9I cut the sequence.

```
[enzymes sites] = rebasecuts(seq, {'CfoI','Tru9I'})
```

4 Search for any possible enzymes that cut after base 7.

```
enzymes  = rebasecuts(seq, 7)
```

5 Get the subset of enzymes that cut between base 11 and 37.

```
enzymes  = rebasecuts(seq, [11 37])
```

See Also

Bioinformatics Toolbox functions: cleave, restrict, seq2regexp, seqshowwords

MATLAB function: regexp

redgreencmap

Purpose

Create red and green color map

Syntax

```
redgreencmap(Length)
redgreencmap(..., 'Interpolation', InterpolationValue, ...)
```

Arguments

Length	Length of the color map. Enter either 256 or 64. Default is the length of the color map of the current figure.
InterpolationValue	Property that lets you set the algorithm for color interpolation. Choices are: • 'linear' • 'quadratic' • 'cubic' • 'sigmoid' (default) **Note** The sigmoid interpolation is tanh.

Description

`redgreencmap(Length)` returns an *Length*-by-3 matrix containing a red and green color map. Low values are bright green, values in the center of the map are black, and high values are red. Enter either 256 or 64 for *Length*. If *Length* is empty, the length of the map will be the same as the length of the color map of the current figure.

`redgreencmap(..., 'PropertyName', PropertyValue, ...)` defines optional properties that use property name/value pairs in any order. These property name/value pairs are as follows:

`redgreencmap(..., 'Interpolation', InterpolationValue, ...)` lets you set the algorithm for color interpolation. Choices are:

- 'linear'

- `'quadratic'`
- `'cubic'`
- `'sigmoid'` (default)

Note The sigmoid interpolation is tanh.

Examples

Reset the color map of the current figure.

```
pd =gprread('mouse_a1pd.gpr')
maimage(pd,'F635 Median')
colormap(redgreencmap)
```

See Also

Bioinformatics Toolbox function: `clustergram`

MATLAB functions: `colormap`, `colormapeditor`

Purpose

Split nucleotide sequence at restriction site

Syntax

```
Fragments = restrict(SeqNT, Enzyme)
Fragments = restrict(SeqNT, Pattern, Position)
[Fragments, CuttingSites] = restrict(...)
[Fragments, CuttingSites, Lengths] = restrict(...)
... = restrict(..., 'PartialDigest', PartialDigestValue)
```

Arguments

SeqNT	Nucleotide sequence. Enter either a character string with the characters A, T, G, C, and ambiguous characters R, Y, K, M, S, W, B, D, H, V, N, or a vector of integers. You can also enter a structure with the field Sequence.
Enzyme	Enter the name of a restriction enzyme from REBASE Version 412.
Pattern	Enter a short nucleotide pattern. Pattern can be a regular expression.
Position	Defines the position on Pattern where the sequence is cut. Position=0 corresponds to the 5' end of the Pattern.
PartialDigestValue	Property to specify a probability for partial digestion. Enter a value from 0 to 1.

Description

Fragments = restrict(*SeqNT*, *Enzyme*) cuts a sequence (*SeqNT*) into fragments at the restriction sites of a restriction enzyme (*Enzyme*). The returned values are stored in a cell array of sequences (*Fragments*).

Fragments = restrict(*SeqNT*, *Pattern*, *Position*) cuts a sequence (*SeqNT*) into fragments at restriction sites specified by a nucleotide pattern (*Pattern*).

[*Fragments, CuttingSites*] = restrict(...) returns a numeric vector with the indices representing the cutting sites. A 0 (zero) is added to the list so numel(*Fragments*)==numel(*CuttingSites*). You can use `CuttingSites+1` to point to the first base of every fragment respective to the original sequence.

`[Fragments, CuttingSites, Lengths] = restrict(...)` returns a numeric vector with the lengths of every fragment.

`... = restrict(..., 'PartialDigest', PartialDigestValue)` simulates a partial digest where each restriction site in the sequence has a probability (*PartialDigestValue*) of being cut.

REBASE, the restriction enzyme database, is a collection of information about restriction enzymes and related proteins. For more information about REBASE or to search REBASE for the name of a restriction enzyme, go to the REBASE Web site at

```
http://rebase.neb.com/rebase/rebase.html
```

Examples

1 Enter a nucleotide sequence.

```
Seq = 'AGAGGGGTACGCGCTCTGAAAAGCGGGAACCTCGTGGCGCTTTATTAA';
```

2 Use the recognition pattern (sequence) `GCGC` with the point of cleavage at position `3` to cleave a nucleotide sequence.

```
fragmentsPattern = restrict(Seq,'GCGC',3)

fragmentsPattern =
    'AGAGGGGTACGCG'
    'CTCTGAAAAGCGGGAACCTCGTGGCG'
    'CTTTATTAA'
```

3 Use the restriction enzyme `HspAI` (recognition sequence `GCGC` with the point of cleavage at position `1`) to cleave a nucleotide sequence.

```
fragmentsEnzyme = restrict(Seq,'HspAI')

fragmentsEnzyme =
    'AGAGGGGTACG'
    'CGCTCTGAAAAGCGGGAACCTCGTGG'
    'CGCTTTATTAA'
```

4 Use a regular expression for the enzyme pattern.

```
fragmentsRegExp = restrict(Seq,'GCG[^C]',3)

fragmentsRegExp =

    'AGAGGGGTACGCGCTCTGAAAAGCG'
    'GGAACCTCGTGGCGCTTTATTAA'
```

5 Capture the cutting sites and fragment lengths with the fragments.

```
[fragments, cut_sites, lengths] = restrict(Seq,'HspAI')

fragments =
    'AGAGGGGTACG'
    'CGCTCTGAAAAGCGGGAACCTCGTGG'
    'CGCTTTATTAA'

cut_sites =
     0
    11
    37

lengths =
    11
    26
    11
```

See Also

Bioinformatics Toolbox functions: `cleave`, `rebasecuts`, `seq2regexp`, `seqshowwords`

MATLAB function: `regexp`

Purpose

Reverse mapping for genetic code

Syntax

```
map = revgeneticcode
revgeneticcode(GeneticCode)
revgeneticcode(..., 'Alphabet', AlphabetValue, ...)
revgeneticcode(..., 'ThreeLetterCodes',
ThreeLetterCodesValue,
   ...)
```

Arguments

GeneticCode	Genetic code for translating nucleotide codons to amino acids. Enter a code number or code name from the table . If you use a code name, you can truncate the name to the first two characters of the name.
AlphabetValue	Property to select the nucleotide alphabet. Enter either `'dna'` or `'rna'`. The default value is `'dna'`.
ThreeLetterCodesValue	Property to select one- or three-letter amino acid codes. Enter `true` for three-letter codes or `false` for one-letter codes.

Genetic Code

Code Number	Code Name
1	Standard
2	Vertebrate Mitochondrial
3	Yeast Mitochondrial
4	Mold, Protozoan, Coelenterate Mitochondrial, and Mycoplasma/Spiroplasma
5	Invertebrate Mitochondrial

Code Number	Code Name
6	Ciliate, Dasycladacean, and Hexamita Nuclear
9	Echinoderm Mitochondrial
10	Euplotid Nuclear
11	Bacterial and Plant Plastid
12	Alternative Yeast Nuclear
13	Ascidian Mitochondrial
14	Flatworm Mitochondrial
15	Blepharisma Nuclear
16	Chlorophycean Mitochondrial
21	Trematode Mitochondrial
22	Scenedesmus Obliquus Mitochondrial
23	Thraustochytrium Mitochondrial

Description

`map = revgeneticcode` returns a structure containing the reverse mapping for the standard genetic code.

`revgeneticcode(GeneticCode)` returns a structure containing the reverse mapping for an alternate genetic code.

`revgeneticcode(..., 'PropertyName', PropertyValue, ...)` calls `revgeneticcode` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`revgeneticcode(..., 'Alphabet', AlphabetValue, ...)` defines the nucleotide alphabet to use in the map.

`revgeneticcode(..., 'ThreeLetterCodes', ThreeLetterCodesValue, ...)` returns the mapping structure with three-letter amino acid codes as field names instead of the default single-letter codes if ThreeLetterCodes is true.

Examples

```
moldcode = revgeneticcode(4,'Alphabet','rna');
wormcode = revgeneticcode('Flatworm Mitochondrial',...
                          'ThreeLetterCodes',true);

map = revgeneticcode

map =

       Name: 'Standard'
          A: {'GCT'  'GCC'  'GCA'  'GCG'}
          R: {'CGT'  'CGC'  'CGA'  'CGG'  'AGA'  'AGG'}
          N: {'AAT'  'AAC'}
          D: {'GAT'  'GAC'}
          C: {'TGT'  'TGC'}
          Q: {'CAA'  'CAG'}
          E: {'GAA'  'GAG'}
          G: {'GGT'  'GGC'  'GGA'  'GGG'}
          H: {'CAT'  'CAC'}
          I: {'ATT'  'ATC'  'ATA'}
          L: {'TTA'  'TTG'  'CTT'  'CTC'  'CTA'  'CTG'}
          K: {'AAA'  'AAG'}
          M: {'ATG'}
          F: {'TTT'  'TTC'}
          P: {'CCT'  'CCC'  'CCA'  'CCG'}
          S: {'TCT'  'TCC'  'TCA'  'TCG'  'AGT'  'AGC'}
          T: {'ACT'  'ACC'  'ACA'  'ACG'}
          W: {'TGG'}
          Y: {'TAT'  'TAC'}
          V: {'GTT'  'GTC'  'GTA'  'GTG'}
      Stops: {'TAA'  'TAG'  'TGA'}
     Starts: {'TTG'  'CTG'  'ATG'}
```

References

[1] NCBI Web page describing genetic codes:

```
http://www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=c
```

See Also

Bioinformatics Toolbox functions: `aa2nt`, `aminolookup`, `baselookup`, `geneticcode`, `nt2aa`

Purpose

Perform background adjustment on Affymetrix microarray probe-level data using Robust Multi-array Average (RMA) procedure

Syntax

```
BackgroundAdjustedMatrix = rmabackadj(PMData)
BackgroundAdjustedMatrix = rmabackadj(..., 'Method',
MethodValue, ...)
BackgroundAdjustedMatrix = rmabackadj(..., 'Truncate',
   TruncateValue, ...)
BackgroundAdjustedMatrix = rmabackadj(..., 'Showplot',
   ShowplotValue, ...)
```

Arguments

PMData	Matrix of intensity values where each row corresponds to a perfect match (PM) probe and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)
MethodValue	Property to control the estimation method for the background adjustment model parameters. Enter either `'RMA'` (to use estimation method described by Bolstad, 2005) or `'MLE'` (to estimate the parameters using maximum likelihood). Default is `'RMA'`.

TruncateValue	Property to control the background noise model. Enter either `true` (use a truncated Gaussian distribution) or `false` (use a nontruncated Gaussian distribution). Default is `true`.
ShowplotValue	Property to control the plotting of a histogram showing the distribution of PM probe intensity values (blue) and the convoluted probability distribution function (red), with estimated parameters. Enter either `'all'` (plot a histogram for each column or chip) or specify a subset of columns (chips) by entering the column number, list of numbers, or range of numbers. For example: • `..., 'Showplot', 3, ...)` plots the intensity values in column 3. • `..., 'Showplot', [3,5,7], ...)` plots the intensity values in columns 3, 5, and 7. • `..., 'Showplot', 3:9, ...)` plots the intensity values in columns 3 to 9.

Description

BackgroundAdjustedMatrix = rmabackadj(*PMData*) returns the background adjusted values of probe intensities in the matrix, *PMData*. Note that each row in *PMData* corresponds to a perfect match (PM) probe and each column in *PMData* corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.) Details on the background adjustment are described by Bolstad, 2005.

BackgroundAdjustedMatrix = rmabackadj(..., '*PropertyName*', *PropertyValue*, ...) defines optional properties that use property name/value pairs in any order. These property name/value pairs are as follows:

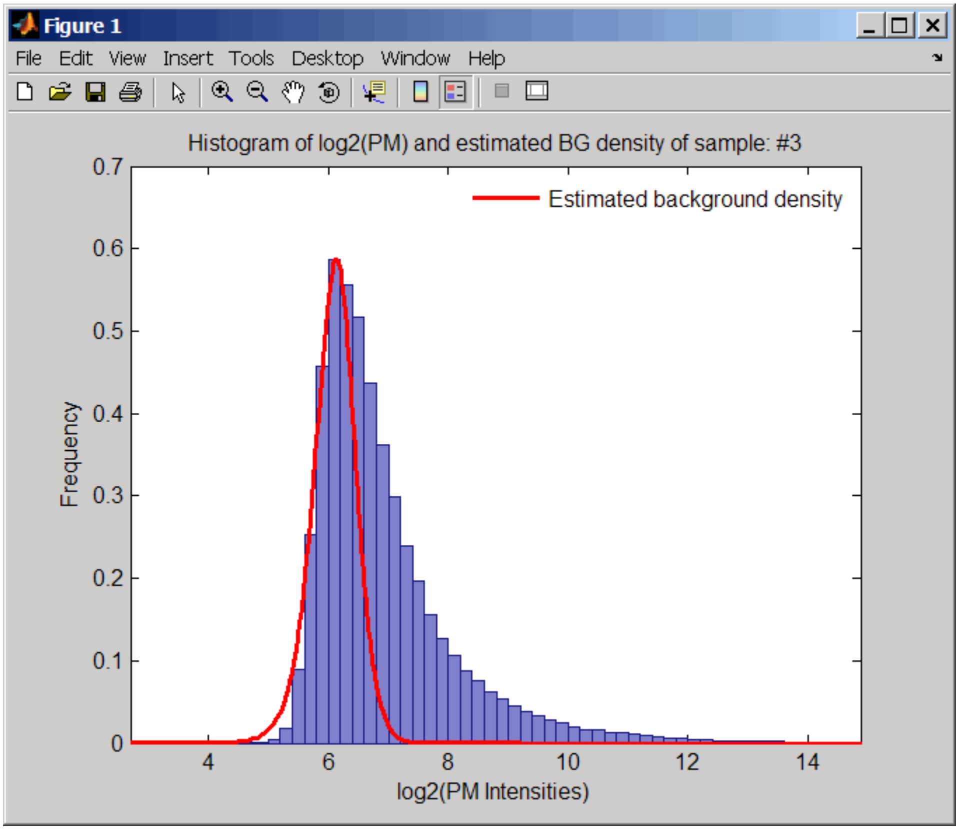
BackgroundAdjustedMatrix = rmabackadj(..., 'Method', *MethodValue*, ...) controls the estimation method for the background adjustment model parameters. When *MethodValue* is 'RMA', rmabackadj implements the estimation method described by Bolstad, 2005. When *MethodValue* is 'MLE', rmabackadj estimates the parameters using maximum likelihood. Default is 'RMA'.

BackgroundAdjustedMatrix = rmabackadj(..., 'Truncate', *TruncateValue*, ...) controls the background noise model used. When *TruncateValue* is false, rmabackadj uses nontruncated Gaussian as the background noise model. Default is true.

BackgroundAdjustedMatrix = rmabackadj(..., 'Showplot', *ShowplotValue*, ...) lets you plot a histogram showing the distribution of PM probe intensity values (blue) and the convoluted probability distribution function (red), with estimated parameters. When *ShowplotValue* is 'all', rmabackadj plots a histogram for each column or chip. When *ShowplotValue* is a number, list of numbers, or range of numbers, rmabackadj plots a histogram for the indicated column number (chip).

For example:

- ..., 'Showplot', 3,...) plots the intensity values in column 3 of *Data*.
- ..., 'Showplot', [3,5,7],...) plots the intensity values in columns 3, 5, and 7 of *Data*.
- ..., 'Showplot', 3:9,...) plots the intensity values in columns 3 to 9 of *PMData*.



Examples

1 Load a MAT file, included with Bioinformatics Toolbox, which contains Affymetrix probe-level data, including `pmMatrix`, a matrix of PM probe intensity values from multiple CEL files.

```
load prostatecancerrawdata
```

2 Perform background adjustment on the PM probe intensity values in the matrix, `pmMatrix`, creating a new matrix, `BackgroundAdjustedMatrix`.

```
BackgroundAdjustedMatrix = rmabackadj(pmMatrix);
```

3 Perform background adjustment on the PM probe intensity values in only column 3 of the matrix, `pmMatrix`, creating a new matrix, `BackgroundAdjustedChip3`.

```
BackgroundAdjustedChip3 = rmabackadj(pmMatrix(:,3));
```

The `prostatecancerrawdata.mat` file used in the previous example contains data from Best et al., 2005.

References

[1] Irizarry, R.A., Hobbs, B., Collin, F., Beazer-Barclay, Y.D., Antonellis, K.J., Scherf, U., Speed, T.P. (2003). Exploration, Normalization, and Summaries of High Density Oligonucleotide Array Probe Level Data. Biostatistics *4*, 249-264.

[2] Bolstad, B. (2005). "affy: Built-in Processing Methods" http://www.bioconductor.org/repository/devel/vignette/builtinMethods.pdf

[3] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823-6834.

See Also

`affyinvarsetnorm`, `affyread`, `celintensityread`, `probelibraryinfo`, `probesetlink`, `probesetlookup`, `probesetvalues`, `quantilenorm`, `rmasummary`

Purpose

Calculate gene (probe set) expression values from Affymetrix microarray probe-level data using Robust Multi-array Average (RMA) procedure

Syntax

```
ExpressionMatrix = rmasummary(ProbeIndices, Data)
ExpressionMatrix = rmasummary(..., 'Output', OutputValue)
```

Arguments

ProbeIndices	Column vector of probe indices. The convention for probe indices is, for each probe set, to label each probe 0 to N - 1, where N is the number of probes in the probe set.
Data	Matrix of natural-scale intensity values where each row corresponds to a perfect match (PM) probe and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)
OutputValue	Property to control the scale of the returned gene expression values. *OutputValue* can be: • `'log'` • `'log2'` • `'log10'` • `'natural'` • `@`*functionname* In the last instance, the data is transformed as defined by the function *functionname*. Default is `'log2'`.

Description

ExpressionMatrix = `rmasummary(`*ProbeIndices*, *Data*`)` returns gene (probe set) expression values after calculating them from natural-scale probe intensities in the matrix *Data*, using the column vector of probe indices, `ProbeIndices`. Note that each row in `Data` corresponds to a perfect match (PM) probe, and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.) Note that the column vector `ProbeIndices` designates probes within each probe set by labeling each probe 0 to N - 1, where N is the number of probes in the probe set. Note that each row in `ExpressionMatrix` corresponds to a gene (probe set) and each column in `ExpressionMatrix` corresponds to an Affymetrix CEL file, which represents a single chip.

For a given probe set n, with J probe pairs, let $Yijn$ denote the background adjusted, base 2 log transformed and quantile-normalized PM probe intensity value of chip i and probe j. $Yijn$ follows a linear additive model:

$$Yijn = Uin + Ajn + Eijn;\ i = 1, ..., I;\ j = 1, ..., J;\ n = 1, ..., N$$

where:

Uin = gene expression of the probe set n on chip i

Ajn = probe affinity effect for the jth probe in the probe set

$Eijn$ = residual for the jth probe on the ith chip

The RMA methods assumes $A1 + A2 + ... + AJ = 0$ for all probe sets. A robust procedure, median polish, is used to estimate Ui as the log scale measure of expression.

Note There is no column in `ExpressionMatrix` that contains probe set or gene information.

`ExpressionMatrix = rmasummary(..., 'PropertyName', PropertyValue, ...)` defines optional properties that use property name/value pairs in any order. These property name/value pairs are as follows:

`ExpressionMatrix = rmasummary(..., 'Output', OutputValue)` controls the scale of the returned gene expression values. `OutputValue` can be:

- `'log'`
- `'log2'`
- `'log10'`
- `'natural'`
- `@functionname`

In the last instance, the data is transformed as defined by the function `functionname`. Default is `'log2'`.

Examples

1 Load a MAT file, included with Bioinformatics Toolbox, which contains Affymetrix data variables, including `pmMatrix`, a matrix of PM probe intensity values from multiple CEL files.

```
load prostatecancerrawdata
```

2 Perform background adjustment on the PM probe intensity values in the matrix, `pmMatrix`, using the `rmabackadj` function, thereby creating a new matrix, `BackgroundAdjustedMatrix`.

```
BackgroundAdjustedMatrix = rmabackadj(pmMatrix);
```

3 Normalize the data in `BackgroundAdjustedMatrix`, using the `quantilenorm` function.

```
NormMatrix = quantilenorm(BackgroundAdjustedMatrix);
```

4 Calculate gene expression values from the probe intensities in `NormMatrix`, creating a new matrix, `ExpressionMatrix`. (You will use the `probeIndices` column vector provided to supply information on the probe indices.)

```
ExpressionMatrix = rmasummary(probeIndices, NormMatrix);
```

The `prostatecancerrawdata.mat` file used in the previous example contains data from Best et al., 2005.

References

[1] Irizarry, R.A., Hobbs, B., Collin, F., Beazer-Barclay, Y.D., Antonellis, K.J., Scherf, U., Speed, T.P. (2003). Exploration, Normalization, and Summaries of High Density Oligonucleotide Array Probe Level Data. Biostatistics. *4*, 249-264.

[2] Mosteller, F., and Tukey, J. (1977). Data Analysis and Regression (Reading, Massachusetts: Addison-Wesley Publishing Company), pp. 165-202.

[3] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823-6834.

See Also

`affyinvarsetnorm`, `celintensityread`, `mainvarsetnorm`, `malowess`, `manorm`, `quantilenorm`, `rmabackadj`

Purpose

Convert RNA sequence of nucleotides to DNA sequence

Syntax

`SeqDNA = rna2dna(SeqRNA)`

Arguments

SeqRNA	Nucleotide sequence for RNA. Enter a character string with the characters `A`, `C`, `U`, `G`, and the ambiguous nucleotide bases `N`, `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, and `V`.

Description

`SeqDNA = rna2dna(SeqRNA)` converts any uracil nucleotides in an RNA sequence into thymine (`U-->T`), and returns in the same format as DNA. For example, if the RNA sequence is an integer sequence then so is *SeqRNA*.

Example

```
rna2dna('ACGAUGAGUCAUGCUU')

ans =
ACGATGAGTCATGCTT
```

See Also

Bioinformatics Toolbox function: `dna2rna`

MATLAB functions: `strrep`, `regexp`

Purpose

Read trace data from SCF file

Syntax

```
Sample = scfread('File')
[Sample, Probability] = scfread('File')
[Sample, Probability, Comments] = scfread('File')
[A, C, T, G] = scfread ('File')
[A, C, T, G, ProbA, ProbC, ProbG, ProbT] = scfread ('File')
[A, C, T, G, ProbA, ProbC, ProbG, ProbT, Comments, PkIndex,
    Base] = scfread ('File')
```

Arguments

File	SCF formatted file. Enter a file name or a path and file name.

Description

`scfread` reads data from an SCF formatted file into MATLAB structures.

`Sample = scfread('File')` reads an SCF formatted file and returns the sample data in the structure `Sample`, which contains the following fields:

Field	Description
`A`	Column vector containing intensity of A fluorescence tag
`C`	Column vector containing intensity of C fluorescence tag
`G`	Column vector containing intensity of G fluorescence tag
`T`	Column vector containing intensity of T fluorescence tag

`[Sample, Probability] = scfread('File')` also returns the probability data in the structure `Probability`, which contains the following fields:

Field	Description
peak_index	Column vector containing the position in the SCF file for the start of the data for each peak
prob_A	Column vector containing the probability of each base in the sequence being an A
prob_C	Column vector containing the probability of each base in the sequence being a C
prob_G	Column vector containing the probability of each base in the sequence being a G
prob_T	Column vector containing the probability of each base in the sequence being a T
base	Column vector containing the called bases for the sequence

`[`*`Sample, Probability, Comments`*`] = scfread('`*`File`*`')` also returns the comment information from the SCF file in a character array `Comments`.

`[`*`A, C, T, G`*`] = scfread ('`*`File`*`')` returns the sample data for the four bases in separate variables.

`[`*`A, C, T, G, ProbA, ProbC, ProbG, ProbT`*`] = scfread ('`*`File`*`')` also returns the probabilities data for the four bases in separate variables.

`[`*`A, C, T, G, ProbA, ProbC, ProbG, ProbT, Comments, PkIndex, Base`*`] = scfread ('`*`File`*`')` also returns the peak indices and called bases in separate variables.

SCF files store data from DNA sequencing instruments. Each file includes sample data, sequence information, and the relative probabilities of each of the four bases. For more information on SCF files, see

```
http://www.mrc-lmb.cam.ac.uk/pubseq/manual/formats_unix_2.html
```

Examples

```
[sampleStruct, probStruct, Comments] = scfread('sample.scf')
sampleStruct =

    A: [10827x1 double]
    C: [10827x1 double]
    G: [10827x1 double]
    T: [10827x1 double]


probStruct =

    peak_index: [742x1 double]
        prob_A: [742x1 double]
        prob_C: [742x1 double]
        prob_G: [742x1 double]
        prob_T: [742x1 double]
          base: [742x1 char]


Comments =

SIGN=A=121,C=103,G=119,T=82
SPAC= 16.25
PRIM=0
MACH=Arkansas_SN312
DYEP=DT3700POP5{BD}v2.mob
NAME=HCIUP1D61207
LANE=6
GELN=
PROC=
RTRK=
CONV=phred version=0.990722.h
COMM=
SRCE=ABI 373A or 377
```

See Also

Bioinformatics Toolbox functions: `genbankread`, `traceplot`

Purpose

Convert sequence with ambiguous characters to regular expression

Syntax

```
seq2regexp(Seq)
seq2regexp(..., 'PropertyName', PropertyValue,...)
seq2regexp(..., 'Alphabet', AlphabetValue)
seq2regexp(..., 'Ambiguous', AmbiguousValue)
```

Arguments

Seq	Amino acid or nucleotide sequence as a string of characters. You can also enter a structure with the field `Sequence`.
AlphabetValue	Property to select the sequence alphabet. Enter either `'AA'` for amino acids or `'NT'` for nucleotides. The default value is `'NT'`.
AmbiguousValue	Property to control returning ambiguous characters in the regular expression. Enter either `true` (include ambiguous characters) or `false` (return only unambiguous characters). The default value is `true`.

Nucleotide Conversions

Nucleotide Letter	Nucleotide	Nucleotide Letter	Nucleotide
A—A	Adenosine	S—[GC]	(Strong)
C—C	Cytosine	W—[AT]	(Weak)
G—G	Guanine	B—[GTC]	
T—T	Thymidine	D—[GAT]	
U—U	Uridine	H—[ACT]	
R—[GA]	(Purine)	V—[GCA]	
Y—[TC]	(Pyrimidine)	N—[AGCT]	Any nucleotide

Nucleotide Letter	Nucleotide	Nucleotide Letter	Nucleotide
K—[GT]	(Keto)	- — -	Gap of indeterminate length
M—[AC]	(Amino)	?—?	Unknown

Amino Acid Conversion

Amino Acid Letter	Description
B—[DN]	Aspartic acid or asparagine
Z—[EQ]	Glutamic acid or glutamine
X—[ARNDCQEGHILKMFPSTWYV]	Any amino acid

Description

`seq2regexp(`*`Seq`*`)` converts ambiguous nucleotide or amino acid symbols in a sequence into a regular expression format using IUB/IUPAC codes.

`seq2regexp(..., '`*`PropertyName`*`', `*`PropertyValue`*`,...)` defines optional properties using property name/value pairs.

`seq2regexp(..., 'Alphabet', `*`AlphabetValue`*`)` selects the sequence alphabet for nucleotide sequences or amino acid sequences.

`seq2regexp(..., 'Ambiguous', `*`AmbiguousValue`*`)`, when *`AmbiguousValue`* is false, removes the ambiguous characters from the output regular expressions. For example:

- If *`Seq`* `= 'ACGTK'`, and *`AmbiguousValue`* is `true` (default), MATLAB returns `ACGT[GTK]` with the unambiguous characters `G` and `T`, and the ambiguous character `K`.
- If *`Seq`* `= 'ACGTK'`, and *`AmbiguousValue`* is `false`, MATLAB returns `ACGT[GT]` with only the unambiguous characters.

Example

1 Convert a nucleotide sequence into a regular expression.

```
seq2regexp('ACWTMAN')

ans =
AC[ATW]T[ACM]A[ACGTRYKMSWBDHVN]
```

2 Remove ambiguous characters from the regular expression.

```
seq2regexp('ACWTMAN', 'ambiguous', false)

ans =
AC[AT]T[AC]A[ACGT]
```

See Also

Bioinformatics Toolbox functions: `restrict`, `seqwordcount`

MATLAB functions: `regexp`, `regexpi`

Purpose

Calculate complementary strand of nucleotide sequence

Syntax

`SeqC = seqcomplement(SeqNT)`

Arguments

SeqNT	Enter either a character string with the characters `A`, `T` (`U`), `G`, `C`, and ambiguous characters `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, `V`, `N`, or a vector of integers. You can also enter a structure with the field `Sequence`.

Description

`SeqC = seqcomplement(SeqNT)` calculates the complementary strand (`A-->T`, `C-->G`, `G-->C`, `T-->A`) of a DNA sequence and returns a sequence in the same format as `SeqNT`. For example, if *SeqNT* is an integer sequence then so is *SeqC*.

Example

Return the complement of a DNA nucleotide sequence.

```
s = 'ATCG';
seqcomplement(s)

ans =
TAGC
```

See Also

Bioinformatics Toolbox functions `seqrcomplement`, `seqreverse`, `seqtool`

seqconsensus

Purpose

Calculate consensus sequence

Syntax

```
CSeq = seqconsensus(Seqs)
[CSeq, Score] = seqconsensus(Seqs)
CSeq = seqconsensus(Profile)
seqconsensus(..., 'PropertyName', PropertyValue,...)
seqconsensus(..., 'ScoringMatrix',  ScoringMatrixValue)
```

Arguments

Seqs	Set of multiply aligned amino acid or nucleotide sequences. Enter an array of strings, a cell array of strings, or an array of structures with the field `Sequence`.
Profile	Sequence profile. Enter a profile from the function `seqprofile`. `Profile` is a matrix of size `[20 (or 4) x Sequence Length]` with the frequency or count of amino acids (or nucleotides) for every position. `Profile` can also have 21 (or 5) rows if gaps are included in the consensus.
ScoringMatrixValue	Scoring matrix. The default value is `BLOSUM50` for amino acid sequences or `NUC44` for nucleotide sequences. `ScoringMatrix` can also be a `21x21`, `5x5`, `20x20`, or `4x4` numeric array. For the gap-included cases, gap scores (last row/column) are set to `mean(diag(ScoringMatrix))`for a gap matching with another gap, and set to `mean(nodiag(ScoringMatrix))` for a gap matching with another symbol

Description

`CSeq = seqconsensus(Seqs)`, for a multiply aligned set of sequences (*Seqs*), returns a string with the consensus sequence (*CSeq*). The frequency of symbols (`20` amino acids, `4` nucleotides) in the set of sequences is determined with the function `seqprofile`. For ambiguous nucleotide or amino acid symbols, the frequency or count is added to the standard set of symbols.

`[CSeq, Score] = seqconsensus(Seqs)` returns the conservation score of the consensus sequence. Scores are computed with the scoring matrix `BLOSUM50` for amino acids or `NUC44` for nucleotides. Scores are the average euclidean distance between the scored symbol and the M-dimensional consensus value. `M` is the size of the alphabet. The consensus value is the profile weighted by the scoring matrix.

`CSeq = seqconsensus(Profile)` returns a string with the consensus sequence (`CSeq`) from a sequence profile (`Profile`).

`seqconsensus(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`seqconsensus(..., 'ScoringMatrix', ScoringMatrixValue)` specifies the scoring matrix.

The following input parameters are analogous to the function `seqprofile` when the alphabet is restricted to `'AA'` or `'NT'`.

`seqconsensus(..., 'Alphabet', AlphabetValue)`

`seqconsensus(..., 'Gaps', GapsValue)`

`seqconsensus(..., 'Ambiguous', AmbiguousValue)`

`seqconsensus(..., 'Limits', LimitsValue)`

Examples

```
seqs = fastaread('pf00002.fa');
[C,S] = seqconsensus(seqs,'limits',[50 60],'gaps','all')
```

See Also

Bioinformatics Toolbox functions `fastaread`, `multialignread`, `profalign`, `seqdisp`, `seqprofile`

Purpose

Format long sequence output for easy viewing

Syntax

```
seqdisp(Seq)
seqdisp(..., 'PropertyName', PropertyValue,...)
seqdisp(..., 'Row', RowValue)
seqdisp(..., 'Column', ColumnValue)
seqdisp(..., 'ShowNumbers', ShowNumbersValue)
```

Arguments

Seq	Nucleotide or amino acid sequence. Enter a character array, a FASTA file name, or a MATLAB structure with the field `Sequence`. Multiply aligned sequences are allowed. FASTA files can have the file extension `fa`, `fasta`, `fas`, `fsa`, or `fst`.
Row	Property to select the length of each row. Enter an integer. The default length is `60`.
Column	Property to select the column width or number of symbols before displaying a space. Enter an integer. The default column width is `10`.
ShowNumbers	Property to control displaying numbers at the start of each row. Enter either `true` (default) to show numbers or `false` to hide numbers.

Description

`seqdisp(`*`Seq`*`)` displays a sequence (`Seq`) in rows with a default row length of 60 and a default column width of `10`.

`seqdisp(..., '`*`PropertyName`*`', `*`PropertyValue`*`,...)` defines optional properties using property name/value pairs.

`seqdisp(..., 'Row', `*`RowValue`*`)` specifies the length of each row for the displayed sequence.

`seqdisp(..., 'Column', ColumnValue)` specifies the number of letters to display before adding a space. `Row` must be larger than and evenly divisible by `Column`.

`seqdisp(..., 'ShowNumbers', ShowNumbersValue)` when `ShowNumbers` is `false`, turns off the position numbers at the start of each row off.

Examples

Read sequence information from the GenBank database. Display the sequence in rows with 50 letters, and within a row, separate every 10 letters with a space.

```
mouseHEXA = getgenbank('AK080777');
seqdisp(mouseHEXA, 'Row', 50, 'Column', 10)
```

Create and save a FASTA file with two sequences, and then display it.

```
hdr = ['Sequence A'; 'Sequence B'];
seq = ['TAGCTGRCCAAGGCCAAGCGAGCTTN';'ATCGACYGGTTCCGGTTCGCTCGAAN']
fastawrite('local.fa', hdr, seq);
seqdisp('local.fa', 'ShowNumbers', false')

ans =
>Sequence A
 1  TAGCTGRCCA AGGCCAAGCG AGCTTN
>Sequence B
 1  ATCGACYGGT TCCGGTTCGC TCGAAN
```

See Also

Bioinformatics Toolbox functions: `multialignread`, `seqconsensus`, `seqlogo`, `seqprofile`, `seqshoworfs`, `seqshowwords`, `seqtool`, `getgenbank`

seqdotplot

Purpose Create dot plot of two sequences

Syntax

```
seqdotplot (Seq1, Seq2)
seqdotplot(Seq1,Seq2, Window, Number)
Matches = seqdotplot(...)
[Matches, Matrix] = seqdotplot(...)
```

Arguments

Seq1, *Seq2*	Nucleotide or amino acid sequences. Enter two character strings. Do not enter a vector of integers. You can also enter a structure with the field `Sequence`.
Window	Enter an integer for the size of a window.
Number	Enter an integer for the number of characters within the window that match.

Description `seqdotplot (`*Seq1*`, `*Seq2*`)` plots a figure that visualizes the match between two sequences.

`seqdotplot(`*Seq1*`,`*Seq2*`, `*Window*`, `*Number*`)` plots sequence matches when there are at least *Number* matches in a window of size *Window*.

When plotting nucleotide sequences, start with a `Window` of `11` and `Number` of `7`.

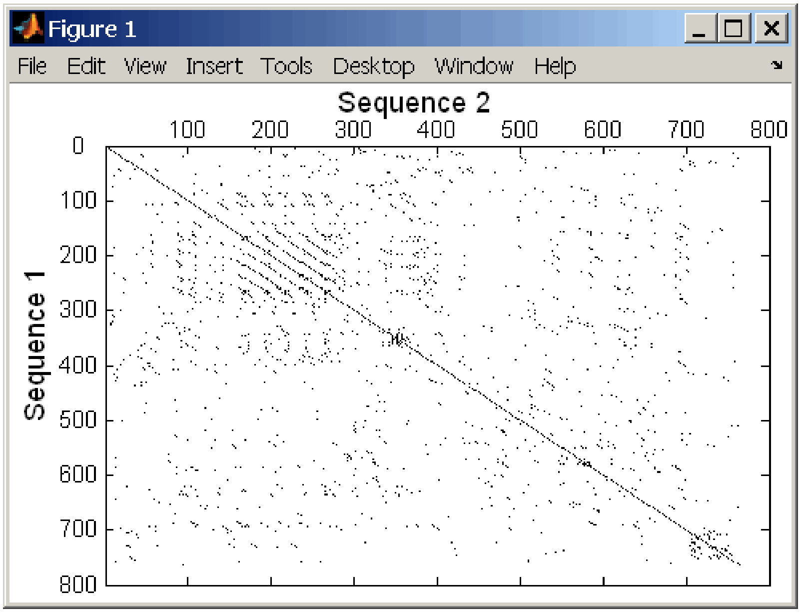
Matches `= seqdotplot(...)` returns the number of dots in the dot plot matrix.

`[`*Matches*`, `*Matrix*`] = seqdotplot(...)` returns the dotplot as a sparse matrix.

Examples This example shows the similarities between the prion protein (PrP) nucleotide sequences of two ruminants, the moufflon and the golden takin.

```
moufflon = getgenbank('AB060288','Sequence',true);
```

```
takin = getgenbank('AB060290','Sequence',true);
seqdotplot(moufflon,takin,11,7)
```




```
Matches = seqdotplot(moufflon,takin,11,7)
Matches =
        5552

[Matches, Matrix] = seqdotplot(moufflon,takin,11,7)
```

See Also

Bioinformatics Toolbox functions `nwalign`, `swalign`

seqinsertgaps

Purpose

Insert gaps into nucleotide or amino acid sequence

Syntax

```
NewSeq = seqinsertgaps(Seq, Positions)
NewSeq = seqinsertgaps(Seq, GappedSeq)
NewSeq = seqinsertgaps(Seq, GappedSeq, Relationship)
```

Arguments

Seq	Either of the following: • String specifying a nucleotide or amino acid sequence • MATLAB structure containing a `Sequence` field
Positions	Vector of integers to specify the positions in *Seq* before which to insert a gap.
GappedSeq	Either of the following: • String specifying a nucleotide or amino acid sequence • MATLAB structure containing a `Sequence` field
Relationship	Integer specifying the relationship between *Seq* and *GappedSeq*. Choices are: • `1` — Both sequences use the same alphabet, that is both are nucleotide sequences or both are amino acid sequences. • `3` — *Seq* contains nucleotides representing codons and *GappedSeq* contains amino acids (default).

Return Values

NewSeq	Sequence with gaps inserted, represented by a string specifying a nucleotide or amino acid sequence.

Description

NewSeq = seqinsertgaps(*Seq*, *Positions*) inserts gaps in the sequence *Seq* before the positions specified by the integers in the vector *Positions*.

NewSeq = seqinsertgaps(*Seq*, *GappedSeq*) finds the gap positions in the sequence *GappedSeq*, then inserts gaps in the corresponding positions in the sequence *Seq*.

NewSeq = seqinsertgaps(*Seq*, *GappedSeq*, *Relationship*) specifies the relationship between *Seq* and *GappedSeq*. Enter 1 for *Relationship* when both sequences use the same alphabet, that is both are nucleotide sequences or both are amino acid sequences. Enter 3 for *Relationship* when *Seq* contains nucleotides representing codons and *GappedSeq* contains amino acids. Default is 3.

Examples

1. Retrieve two nucleotide sequences from the GenBank database for the neuraminidase (NA) protein of two strains of the Influenza A virus (H5N1).

   ```
   hk01 = getgenbank('AF509094');
   vt04 = getgenbank('DQ094287');
   ```

2. Extract the coding region from the two nucleotide sequences.

   ```
   hk01_cds = featuresparse(hk01,'feature','CDS','Sequence',true);
   vt04_cds = featuresparse(vt04,'feature','CDS','Sequence',true);
   ```

3. Align the amino acids sequences converted from the nucleotide sequences.

   ```
   [sc,al]=nwalign(nt2aa(hk01_cds),nt2aa(vt04_cds),'extendgap',1);
   ```

4. Use the seqinsertgaps function to copy the gaps from the aligned amino acid sequences to their corresponding nucleotide sequences, thus codon-aligning them.

   ```
   hk01_aligned = seqinsertgaps(hk01_cds,al(1,:))
   vt04_aligned = seqinsertgaps(vt04_cds,al(3,:))
   ```

5 Once you have code aligned the two sequences, you can use them as input to other functions such as `dnds`, which calculates the synonymous and nonsynonymous substitutions rates of the codon-aligned nucleotide sequences. By setting `Verbose` to `true`, you can also display the codons considered in the computations and their amino acid translations.

```
[dn,ds] = dnds(hk01_aligned,vt04_aligned,'verbose',true)
```

See Also

Bioinformatics Toolbox functions: `dnds`, `dndsml`, `int2aa`, `int2nt`

Purpose

Construct phylogenetic tree from pair-wise distances

Syntax

```
Tree = seqlinkage(Dist)
Tree = seqlinkage(Dist, Method)
Tree = seqlinkage(Dist, Method, Names)
```

Arguments

Dist	Matrix or vector of pair-wise distances, such as returned by the `seqpdist` function.
Method	String that specifies a distance method. Choices are: • `'single'` • `'complete'` • `'average'` (default) • `'weighted'` • `'centroid'` • `'median'`
Names	Property to use alternative labels for leaf nodes. Enter a vector of structures, with the fields `'Header'` or `'Name'`, or a cell array of strings. In both cases the number of elements you provide must comply with the number of samples used to generate the pair-wise distances in *Dist*.

Description

Tree = `seqlinkage(`*Dist*`)` returns a phylogenetic tree object from the pair-wise distances, *Dist*, between the species or products. *Dist* is a matrix or vector of pair-wise distances, such as returned by the `seqpdist` function.

Tree = `seqlinkage(`*Dist*, *Method*`)` creates a phylogenetic tree object using a specified patristic distance method. The available methods are:

`'single'`	Nearest distance (single linkage method)
`'complete'`	Furthest distance (complete linkage method)
`'average'` (default)	Unweighted Pair Group Method Average (UPGMA, group average).
`'weighted'`	Weighted Pair Group Method Average (WPGMA)
`'centroid'`	Unweighted Pair Group Method Centroid (UPGMC)
`'median'`	Weighted Pair Group Method Centroid (WPGMC)

`Tree` `= seqlinkage(`*`Dist`*`,` *`Method`*`,` *`Names`*`)` passes a list of names to label the leaf nodes (for example, species or products) in a phylogenetic tree object.

Examples

```
% Load a multiple alignment of amino acids:
seqs = fastaread('pf00002.fa');
% Measure the 'Jukes-Cantor' pairwise distances:
dist = seqpdist(seqs,'method','jukes-cantor',...
                              'indels','pair');
% Build the phylogenetic tree with the single linkage
% method and pass the names of the sequences:
tree = seqlinkage(dist,'single',seqs)
view(tree)
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreewrite`, `seqpdist`, `seqneighjoin`

Bioinformatics Toolbox methods of phytree object: `plot`, `view`

Purpose Display sequence logo for nucleotide or amino acid sequences

Syntax

```
seqlogo(Seqs)
seqlogo(Profile)
DisplayInfo = seqlogo(Seqs)
seqlogo(..., 'Displaylogo', DisplaylogoValue, ...)
seqlogo(..., 'Alphabet', AlphabetValue, ...)
seqlogo(..., 'Startat', StartatValue, ...)
seqlogo(..., 'Endat', EndatValue, ...)
seqlogo(..., 'SSCorrection', SSCorrectionValue, ...)
```

Arguments

Seqs — Set of pair-wise or multiply aligned nucleotide or amino acid sequences, represented by any of the following:

- Character array
- Cell array of strings
- Array of structures containing a `Sequence` field

Profile — Sequence profile distribution matrix with the frequency of nucleotides or amino acids for every column in the multiple alignment, such as returned by the `seqprofile` function.

The size of the frequency distribution matrix is:

- For nucleotides — `[4 x sequence length]`
- For amino acids — `[20 x sequence length]`

If gaps were included, *`Profile`* may have `5` rows (for nucleotides) or `21` rows (for amino acids), but `seqlogo` ignores gaps.

DisplaylogoValue	Controls the display of a sequence logo. Choices are `true` (default) or `false`.
AlphabetValue	String specifying the type of sequence (nucleotide or amino acid). Choices are `'NT'` (default) or`'AA'`.
StartatValue	Positive integer that specifies the starting position for the sequences in *Seqs*. Default starting position is `1`.
EndatValue	Positive integer that specifies the ending position for the sequences in *Seqs*. Default ending position is the maximum length of the sequences in *Seqs*.
SSCorrectionValue	Controls the use of small sample correction in the estimation of the number of bits. Choices are `true` (default) or `false`.

Return Values

DisplayInfo	Cell array containing the symbol list in *Seqs* and the weight matrix used to graphically display the sequence logo.

Description

`seqlogo(`*`Seqs`*`)` displays a sequence logo for *Seqs*, a set of aligned sequences. The logo graphically displays the sequence conservation at a particular position in the alignment of sequences, measured in bits. The maximum sequence conservation per site is `log2(4)` bits for nucleotide sequences and `log2(20)` bits for amino acid sequences. If the sequence conservation value is zero or negative, no logo is displayed in that position.

`seqlogo(`*`Profile`*`)` displays a sequence logo for *Profile*, a sequence profile distribution matrix with the frequency of nucleotides or amino acids for every column in the multiple alignment, such as returned by the `seqprofile` function.

Color Code for Nucleotides

Nucleotide	Color
A	Green
C	Blue
G	Yellow
T, U	Red
Other	Purple

Color Code for Amino Acids

Amino Acid	Chemical Property	Color
G S T Y C Q N	Polar	Green
A V L I P W F M	Hydrophobic	Orange
D E	Acidic	Red
K R H	Basic	Blue
Other	—	Tan

`DisplayInfo = seqlogo(Seqs)` returns a cell array of unique symbols in a sequence (`Seqs`) and the information weight matrix used to graphically display the logo.

`seqlogo(Seqs, ...'PropertyName', PropertyValue, ...)` calls `seqpdist` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`seqlogo(..., 'Displaylogo', DisplaylogoValue, ...)` controls the display of a sequence logo. Choices are `true` (default) or `false`.

`seqlogo(..., 'Alphabet', AlphabetValue, ...)` specifies the type of sequence (nucleotide or amino acid). Choices are `'NT'` (default) or`'AA'`.

Note If you provide amino acid sequences to `seqlogo`, you must set `Alphabet` to `'AA'`.

`seqlogo(..., 'Startat', StartatValue, ...)` specifies the starting position for the sequences in *`Seqs`*. Default starting position is `1`.

`seqlogo(..., 'Endat', EndatValue, ...)` specifies the ending position for the sequences in *`Seqs`*. Default ending position is the maximum length of the sequences in *`Seqs`*.

`seqlogo(..., 'SSCorrection', SSCorrectionValue, ...)` controls the use of small sample correction in the estimation of the number of bits. Choices are `true` (default) or `false`.

Note A simple calculation of bits tends to overestimate the conservation at a particular location. To compensate for this overestimation, when `SSCorrection` is set to `true`, a rough estimate is applied as an approximate correction. This correction works better when the number of sequences is greater than 50.

Examples

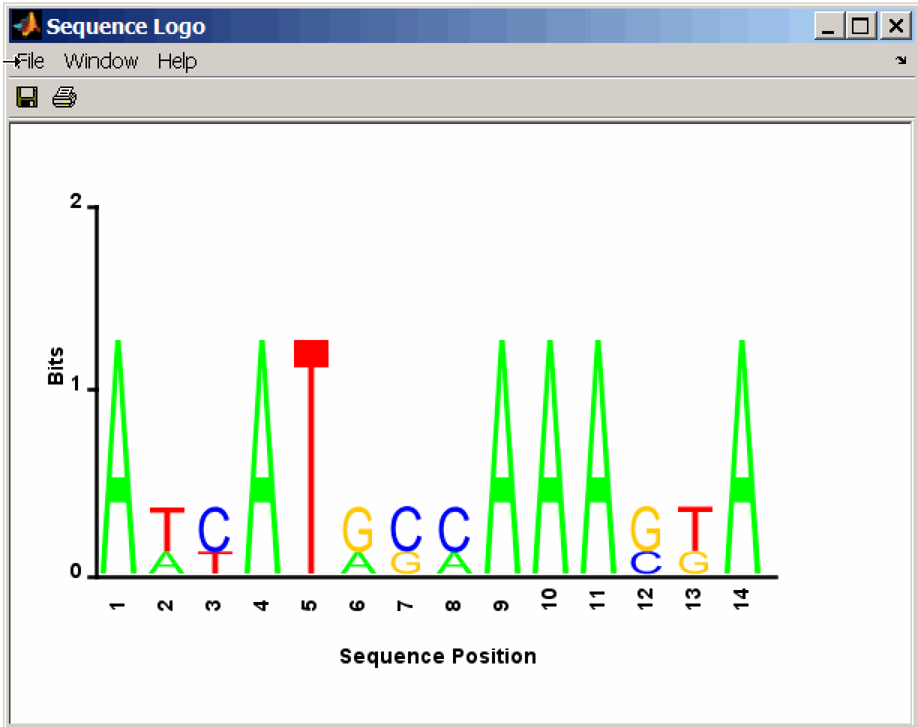
Displaying a Sequence Logo for a Nucleotide Sequence

1 Create a series of aligned nucleotide sequences.

```
S = {'ATTATAGCAAACTA',...
     'AACATGCCAAAGTA',...
     'ATCATGCAAAAGGA'}
```

2 Display the sequence logo.

```
seqlogo(S)
```



3 Notice that correction for small samples prevents you from seeing columns with information equal to `log2(4) = 2` bits, but you can turn this adjustment off.

```
seqlogo(S,'sscorrection',false)
```

Displaying a Sequence Logo for an Amino Acid Sequence

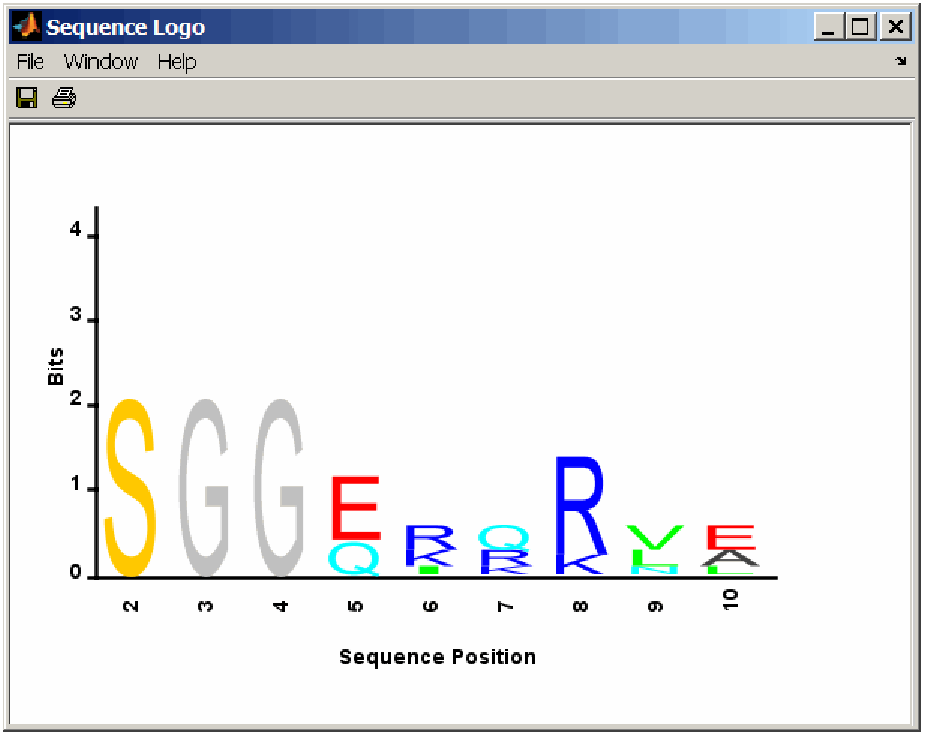
1 Create a series of aligned amino acid sequences.

```
S2 = {'LSGGQRQRVAIARALAL',...
      'LSGGEKQRVAIARALMN',...
```

```
'LSGGQIQRVLLARALAA',...
'LSGGERRRLEIACVLAL',...
'FSGGEKKKNELWQMLAL',...
'LSGGERRRLEIACVLAL'};
```

2 Display the sequence logo, specifying an amino acid sequence and limiting the logo to sequence positions 2 through 10.

```
seqlogo(S2, 'alphabet', 'aa', 'startAt', 2, 'endAt', 10)
```



References

[1] Schneider, T.D., and Stephens, R.M. (1990). Sequence Logos: A new way to display consensus sequences. Nucleic Acids Research *18*, 6097–6100.

See Also

Bioinformatics Toolbox functions: seqconsensus, seqdisp, seqprofile

seqmatch

Purpose Find matches for every string in library

Syntax `Index = seqmatch(Strings, Library)`

Description `Index = seqmatch(Strings, Library)` looks through the elements of `Library` to find strings that begin with every string in `Strings`. `Index` contains the index to the first occurrence for every string in the query. `Strings` and `Library` must be cell arrays of strings.

Examples

```
lib = {'VIPS_HUMAN', 'SCCR_RABIT', 'CALR_PIG' ,'VIPR_RAT', 'PACR_MOUSE'};
query = {'CALR','VIP'};
h = seqmatch(query,lib);
lib(h)
```

See Also MATLAB functions: `regexp`, `strmatch`

Purpose

Neighbor-joining method for phylogenetic tree reconstruction

Syntax

```
Tree = seqneighjoin(Dist)
Tree = seqneighjoin(Dist, Method)
Tree = seqneighjoin(Dist, Method, Names)
seqneighjoin(..., 'PropertyName', PropertyValue,...)
seqneighjoin(..., 'Reroot', RerootValue)
```

Arguments

Dist	Matrix or vector returned by the `seqpdist` function
Method	Method to compute the distances between nodes. Enter `'equivar'` (default), `'firstorder'`, or `'average'`.
Names	Vector of structures with the fields `'Header'`, `'Name'`, or a cell array of strings. In all cases the number of elements must equal the number of samples used to generate the pairwise distances in `Dist`.

Description

`Tree = seqneighjoin(Dist)` computes a phylogenetic tree object from pairwise distances (*Dist*) between the species or products using the neighbor-joining method.

`Tree = seqneighjoin(Dist, Method)` selects a method (*Method*) to compute the distances of the new nodes to all other nodes at every iteration. The general expression to calculate the distances between the new node (`n`), after joining `i` and `j` and all other nodes (`k`), is given by

```
D(n,k) =  a*D(i,k) + (1-a)*D(j,k) - a*D(n,i) - (1-a)*D(n,j)
```

This expression is guaranteed to find the correct tree with additive data (minimum variance reduction).

The following table describes the values for *Method*.

`'equivar'` (default)	Assumes equal variance and independence of evolutionary distance estimates (a = 1/2). Such as in Studier and Keppler, JMBE (1988).
`'firstorder'`	Assumes a first-order model of the variances and covariances of evolutionary distance estimates, `'a'` is adjusted at every iteration to a value between `0` and `1`. Such as in Gascuel, JMBE (1997).
`'average'`	New distances are the weighted average of previous distances while the branch distances are ignored. `D(n,k) =  [ D(i,k) + D(j,k) ] /2` As in the original neighbor-joining algorithm by Saitou and Nei, JMBE (1987).

`Tree = seqneighjoin(`*`Dist`*`, `*`Method`*`, `*`Names`*`)` passes a list of names (*`Names`*) to label the leaf nodes (e.g., species or products) in the phylogenetic tree object.

`seqneighjoin(..., '`*`PropertyName`*`', `*`PropertyValue`*`,...)` defines optional properties using property name/value pairs.

`seqneighjoin(..., 'Reroot', `*`RerootValue`*`)`, when *`RerootValue`* is `false`, excludes rerooting the resulting tree. This is useful for observing the original linkage order followed by the algorithm. By default `seqneighjoin` reroots the resulting tree using the midpoint method.

Examples

1 Load a multiple alignment of amino acids.

```
seqs = fastaread('pf00002.fa');
```

2 Measure the Jukes-Cantor pair-wise distances.

```
dist = seqpdist(seqs,'method','jukes-cantor','indels','pair');
```

3 Build the phylogenetic using the neighbor-joining algorithm.

```
tree = seqneighjoin(dist,'equivar',seqs)
view(tree)
```

References

[1] Saitou, N., and Nei, M. (1987). The neighbor-joining method: A new method for reconstructing phylogenetic trees. Molecular Biology and Evolution *4(4)*, 406–425.

[2] Gascuel, O. (1997). BIONJ: An improved version of the NJ algorithm based on a simple model of sequence data. Molecular Biology and Evolution *14* 685–695.

[3] Studier, J.A., Keppler, K.J. (1988). A note on the neighbor-joining algorithm of Saitou and Nei. Molecular Biology and Evolution *5(6)* 729–731.

See Also

Bioinformatics Toolbox functions: `multialign`, `phytree` (object constructor), `seqlinkage` (alternative method to create a phylogenetic tree), `seqpdist`

Methods of phytree object: `reroot`, `view`

seqpdist

Purpose

Calculate pair-wise distance between sequences

Syntax

```
D = seqpdist(Seqs)
D = seqpdist(Seqs, ...'Method', MethodValue, ...)
D = seqpdist(Seqs, ...'Indels', IndelsValue, ...)
D = seqpdist(Seqs, ...'Optargs', OptargsValue, ...)
D = seqpdist(Seqs, ...'PairwiseAlignment',
   PairwiseAlignmentValue, ...)
D = seqpdist(Seqs, ...'JobManager', JobManagerValue, ...)
D = seqpdist(Seqs, ...'WaitInQueue', WaitInQueueValue, ...)
D = seqpdist(Seqs, ...'SquareForm', SquareFormValue, ...)
D = seqpdist(Seqs, ...'Alphabet', AlphabetValue, ...)
D = seqpdist(Seqs, ...'ScoringMatrix', ScoringMatrixValue,
    ...)
D = seqpdist(Seqs, ...'Scale', ScaleValue, ...)
D = seqpdist(Seqs, ...'GapOpen', GapOpenValue, ...)
D = seqpdist(Seqs, ...'ExtendGap', ExtendGapValue, ...)
```

Arguments

Seqs	Any of the following: • Cell array containing nucleotide or amino acid sequences • Vector of structures containing a `Sequence` field • Matrix of characters, in which each row corresponds to a nucleotide or amino acid sequence
MethodValue	String that specifies the method for calculating pair-wise distances. Default is `Jukes-Cantor`.
IndelsValue	String that specifies how to treat sites with gaps. Default is `score`.

OptargsValue	String or cell array specifying one or more input arguments required or accepted by the distance method specified by the `Method` property.
PairwiseAlignmentValue	Controls the global pair-wise alignment of input sequences (using the `nwalign` function), while ignoring the multiple alignment of the input sequences (if any). Choices are `true` or `false`. Default is: • `true` — When all input sequences do not have the same length. • `false` — When all input sequences have the same length. **Tip** If your input sequences have the same length, `seqpdist` will assume they aligned. If they are not aligned, do one of the following: • Align the sequences before passing them to `seqpdist`, for example, using the `multialign` function. • Set `PairwiseAlignment` to `true` when using `seqpdist`.

JobManagerValue	A `jobmanager object`, such as returned by the Distributed Computing Toolbox function `findResource`, that represents an available distributed MATLAB resource. Specifying this property distributes pair-wise alignments into a cluster of computers using Distributed Computing Toolbox. You must have Distributed Computing Toolbox to use this property.
WaitInQueueValue	Controls whether `seqpdist` waits for a distributed MATLAB resource to be available when you have set the `JobManager` property. Choices are `true` or `false` (default). You must have Distributed Computing Toolbox to use this property.
SquareFormValue	Controls the conversion of the output into a square matrix. Choices are `true` or `false` (default).
AlphabetValue	String specifying the type of sequence (nucleotide or amino acid). Choices are `'NT'` or `'AA'` (default).

ScoringMatrixValue	String specifying the scoring matrix to use for the global pair-wise alignment. Choices for amino acid sequences are: • 'PAM40' • 'PAM250' • 'DAYHOFF' • 'GONNET' • 'BLOSUM30' increasing by 5 up to 'BLOSUM90' • 'BLOSUM62' • 'BLOSUM100' Default is: • 'NUC44' (when *AlphabetValue* equals 'NT') • 'BLOSUM50' (when *AlphabetValue* equals 'AA')
ScaleValue	Positive value that specifies the scale factor used to return the score in arbitrary units. If the scoring matrix information also provides a scale factor, then both are used.
GapOpenValue	Positive integer specifying the penalty for opening a gap in the alignment. Default is 8.
ExtendedGapValue	Positive integer specifying the penalty for extending a gap. Default is equal to *GapOpenValue*.

Return Values

D	Vector containing biological distances between each pair of sequences stored in the M elements of *Seqs*.

Description

D = seqpdist(*Seqs*) returns *D*, a vector containing biological distances between each pair of sequences stored in the M sequences of *Seqs*, a cell array of sequences, a vector of structures, or a matrix or sequences.

D is a 1-by-(M*(M-1)/2) row vector corresponding to the M*(M-1)/2 pairs of sequences in Seqs. The output *D* is arranged in the order ((2,1),(3,1),..., (M,1),(3,2),...(M,2),.....(M,M-1)). This is the lower-left triangle of the full M-by-M distance matrix. To get the distance between the *I*th and the *J*th sequences for I > J, use the formula D((J-1)*(M-J/2)+I-J).

D = seqpdist(*Seqs*, ...'*PropertyName*', *PropertyValue*, ...) calls seqpdist with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

D = seqpdist(*Seqs*, ...'Method', *MethodValue*, ...) specifies a method to compute distances between every pair of sequences. Choices are shown in the following tables.

Methods for Nucleotides and Amino Acids

Method	Description
p-distance	Proportion of sites at which the two sequences are different. p is close to 1 for poorly related sequences, and p is close to 0 for similar sequences. d = p

Method	Description

`Jukes-Cantor` (default)	Maximum likelihood estimate of the number of substitutions between two sequences. `p` is described with the method `p-distance`.For nucleotides:
	`d = -3/4 log(1-p * 4/3)`
	For amino acids:
	`d = -19/20 log(1-p * 20/19)`

`alignment-score`	Distance (`d`) between two sequences (1, 2) is computed from the pair-wise alignment score between the two sequences (`score12`), and the pair-wise alignment score between each sequence and itself (`score11`, `score22`) as follows: `d = (1-score12/score11)* (1-score12/score22)` This option does not imply that prealigned input sequences will be realigned, it only scores them. Use with care; this distance method does not comply with the ultrametric condition. In the rare case where the score between sequences is greater than the score when aligning a sequence with itself, then `d = 0`.

Methods with No Scoring of Gaps (Nucleotides Only)

Method	Description
`Tajima-Nei`	Maximum likelihood estimate considering the background nucleotide frequencies. It can be computed from the input sequences or given by setting `Optargs` to `[gA gC gG gT]`. `gA`, `gC`, `gG`, `gT` are scalar values for the nucleotide frequencies.
`Kimura`	Considers separately the transitional nucleotide substitution and the transversional nucleotide substitution.
`Tamura`	Considers separately the transitional nucleotide substitution, the transversional nucleotide substitution, and the GC content. GC content can be computed from the input sequences or given by setting `Optargs` to the proportion of GC content (scalar value form `0` to `1`).
`Hasegawa`	Considers separately the transitional nucleotide substitution, the transversional nucleotide substitution, and the background nucleotide frequencies. Background frequencies can be computed from the input sequences or given by setting the `Optargs` property to `[gA gC gG gT]`.
`Nei-Tamura`	Considers separately the transitional nucleotide substitution between purines, the transitional nucleotide substitution between pyrimidines, the transversional nucleotide substitution, and the background nucleotide frequencies. Background frequencies can be computed from the input sequences or given by setting the `Optargs` property to `[gA gC gG gT]`.

Methods with No Scoring of Gaps (Amino Acids Only)

Method	Description
`Poisson`	Assumes that the number of amino acid substitutions at each site has a Poisson distribution.
`Gamma`	Assumes that the number of amino acid substitutions at each site has a Gamma distribution with parameter `a`. You can set `a` by using the `Optargs` property. Default is `2`.

You can also specify a user-defined distance function using `@`, for example, `@distfun`. The distance function must be of the form:

```
function D = distfun(S1, S2, OptArgsValue)
```

The `distfun` function takes the following arguments:

- *`S1`* , *`S2`* — Two sequences of the same length (nucleotide or amino acid).
- *`OptArgsValue`* — Optional problem-dependent arguments.

The `distfun` function returns a scalar that represents the distance between *`S1`* and *`S2`*.

`D = seqpdist(Seqs, ...'Indels', IndelsValue, ...)` specifies how to treat sites with gaps. Choices are:

- `score` (default) — Scores these sites either as a point mutation or with the alignment parameters, depending on the method selected.
- `pairwise-del` — For every pair-wise comparison, it ignores the sites with gaps.

- `complete-del` — Ignores all the columns in the multiple alignment that contain a gap. This option is available only if a multiple alignment was provided as the input *Seqs*.

`D = seqpdist(Seqs, ...'Optargs', OptargsValue, ...)` passes one or more arguments required or accepted by the distance method specified by the `Method` property. Use a string or cell array to pass one or multiple input arguments. For example, you can provide the nucleotide frequencies for the `Tajima-Nei` distance method, instead of computing them from the input sequences.

`D = seqpdist(Seqs, ...'PairwiseAlignment', PairwiseAlignmentValue, ...)` controls the global pair-wise alignment of input sequences (using the `nwalign` function), while ignoring the multiple alignment of the input sequences (if any). Default is:

- `true` — When all input sequences do not have the same length.
- `false` — When all input sequences have the same length.

Tip If your input sequences have the same length, `seqpdist` will assume they aligned. If they are not aligned, do one of the following:

- Align the sequences before passing them to `seqpdist`, for example, using the `multialign` function.
- Set `PairwiseAlignment` to `true` when using `seqpdist`.

`D = seqpdist(Seqs, ...'JobManager', JobManagerValue, ...)` distributes pair-wise alignments into a cluster of computers using Distributed Computing Toolbox. *JobManagerValue* is a `jobmanager object` such as returned by the Distributed Computing Toolbox function `findResource`, that represents an available distributed MATLAB resource. You must have Distributed Computing Toolbox to use this property.

D = seqpdist(*Seqs*, ...'WaitInQueue', *WaitInQueueValue*, ...) controls whether seqpdist waits for a distributed MATLAB resource to be available when you have set the JobManager property. When *WaitInQueueValue* is true, seqpdist waits in the job manager queue for an available worker. When *WaitInQueueValue* is false (default) and there are no workers immediately available, seqpdist stops and displays an error message. You must have Distributed Computing Toolbox and have also set the JobManager property to use this property.

D = seqpdist(*Seqs*, ...'SquareForm', *SquareFormValue*, ...), controls the conversion of the output into a square matrix such that *D*(*I*,*J*) denotes the distance between the *I*th and *J*th sequences. The square matrix is symmetric and has a zero diagonal. Choices are true or false (default). Setting Squareform to true is the same as using the squareform function in Statistics Toolbox.

D = seqpdist(*Seqs*, ...'Alphabet', *AlphabetValue*, ...) specifies the type of sequence (nucleotide or amino acid). Choices are 'NT' or 'AA' (default).

The remaining input properties are available when the Method property equals 'alignment-score' or the PairwiseAlignment property equals true.

D = seqpdist(*Seqs*, ...'ScoringMatrix', *ScoringMatrixValue*, ...) specifies the scoring matrix to use for the global pair-wise alignment. Default is:

- 'NUC44' (when *AlphabetValue* equals 'NT')
- 'BLOSUM50' (when *AlphabetValue* equals 'AA')

D = seqpdist(*Seqs*, ...'Scale', *ScaleValue*, ...) specifies the scale factor used to return the score in arbitrary units. Choices are any positive value. If the scoring matrix information also provides a scale factor, then both are used.

D = seqpdist(*Seqs*, ...'GapOpen', *GapOpenValue*, ...) specifies the penalty for opening a gap in the alignment. Choices are any positive integer. Default is 8.

D = seqpdist(*Seqs*, ...'ExtendGap', *ExtendGapValue*, ...) specifies the penalty for extending a gap in the alignment. Choices are any positive integer. Default is equal to *GapOpenValue*.

Examples

1 Read amino acids alignment data into a MATLAB structure.

```
seqs = fastaread('pf00002.fa');
```

2 For every possible pair of sequences in the multiple alignment, ignore sites with gaps and score with the scoring matrix PAM250.

```
dist = seqpdist(seqs,'Method','alignment-score',...
                'Indels','pairwise-delete',...
                'ScoringMatrix','pam250');
```

3 Force the realignment of every pair of sequences ignoring the provided multiple alignment.

```
dist = seqpdist(seqs,'Method','alignment-score',...
                'Indels','pairwise-delete',...
                'ScoringMatrix','pam250',...
                'PairwiseAlignment',true);
```

4 Measure the 'Jukes-Cantor' pair-wise distances after realigning every pair of sequences, counting the gaps as point mutations.

```
dist = seqpdist(seqs,'Method','jukes-cantor',...
                'Indels','score',...
                'Scoringmatrix','pam250',...
                'PairwiseAlignment',true);
```

See Also

Bioinformatics Toolbox functions: fastaread, dnds, dndsml, multialign, nwalign, phytree (object constructor), seqlinkage

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox method of a phytree object: pdist

Purpose

Calculate sequence profile from set of multiply aligned sequences

Syntax

```
Profile = seqprofile(Seqs, 'PropertyName',
   PropertyValue ...)
[Profile, Symbols] = seqprofile(Seqs)
seqprofile(..., 'Alphabet', AlphabetValue)
seqprofile(..., 'Counts', CountsValue)
seqprofile(..., 'Gaps', GapsValue)
seqprofile(..., 'Ambiguous', AmbiguousValue),
seqprofile(..., 'Limits', LimitsValue)
```

Arguments

`Seqs`	Set of multiply aligned sequences. Enter an array of strings, cell array of strings, or an array of structures with the field `Sequence`.
`Alphabet`	Sequence alphabet. Enter `'NT'` (nucleotides), `'AA'` (amino acids), or `'none'`. The default alphabet is `'AA'`. When `Alphabet` is `'none'`, the symbol list is based on the observed symbols. Every character can be a symbol except for a hyphen (-) and a period (.), which are reserved for gaps.
`Count`	Property to control returning frequency (ratio of counts/total counts) or counts. Enter either `true` (counts) or `false` (frequency). The default value is `false`.
`Gaps`	Property to control counting gaps in a sequence. Enter `'all'` (counts all gaps), `'noflanks'` (counts all gaps except those at the flanks of every sequence), or `'none'`. The default value is `'none'`.

`Ambiguous`	Property to control counting ambiguous symbols. Enter `'Count'` to add partial counts to the standard symbols.
`Limits`	Property to specify using part of the sequences. Enter a `[1x2]` vector with the first position and the last position to include in the profile. The default value is `[1,SeqLength]`.

Description

`Profile = seqprofile(Seqs, 'PropertyName', PropertyValue ...)` returns a matrix (`Profile`) of size `[20 (or 4) x SequenceLength]` with the frequency of amino acids (or nucleotides) for every column in the multiple alignment. The order of the rows is given by

- 4 nucleotides — `A C G T/U`
- 20 amino acids — `A R N D C Q E G H I L K M F P S T W Y V`

`[Profile, Symbols] = seqprofile(Seqs)` returns a unique symbol list (`Symbols`) where every symbol in the list corresponds to a row in the profile (`Profile`).

`seqprofile(..., 'Alphabet', AlphabetValue)` selects a nucleotide alphabet, amino acid alphabet, or no alphabet.

`seqprofile(..., 'Counts', CountsValue)` when `Counts` is `true`, returns the counts instead of the frequency.

`seqprofile(..., 'Gaps', GapsValue)` appends a row to the bottom of a profile (`Profile`) with the count for gaps.

`seqprofile(..., 'Ambiguous', AmbiguousValue)`, when `Ambiguous` is `'count'`, counts the ambiguous amino acid symbols (`B Z X`) and nucleotide symbols (`R Y K M S W B D H V N`) with the standard symbols. For example, the amino acid `X` adds a `1/20` count to every row while the amino acid `B` counts as `1/2` at the `D` and `N` rows.

`seqprofile(..., 'Limits', LimitsValue)` specifies the start and end positions for the profile relative to the indices of the multiple alignment.

Examples

```
seqs = fastaread('pf00002.fa');
[P,S] = seqprofile(seqs,'limits',[50 60],'gaps','all')
```

See Also

Bioinformatics Toolbox functions `fastaread`, `multialignread`, `seqconsensus`, `seqdisp`, `seqlogo`

seqrcomplement

Purpose

Calculate reverse complement of nucleotide sequence

Syntax

```
SeqRC = seqrcomplement(SeqNT)
```

Arguments

SeqNT	Nucleotide sequence. Enter either a character string with the characters A, T (U), G, C, and ambiguous characters R, Y, K, M, S, W, B, D, H, V, N, or a vector of integers. You can also enter a structure with the field Sequence.

Description

seqrcomplement calculates the reverse complementary strand of a DNA sequence.

SeqRC = seqrcomplement(SeqNT) calculates the reverse complementary strand 3' --> 5' (A-->T, C-->G, G-->C, T-->A) for a DNA sequence and returns a sequence in the same format as SeqNT. For example, if SeqNT is an integer sequence then so is SeqRC.

Examples

Reverse a DNA nucleotide sequence and then return its complement.

```
s = 'ATCG'
seqrcomplement(s)

ans =
CGAT
```

See Also

Bioinformatics Toolbox functions codoncount, palindromes seqcomplement, seqreverse, seqtool

Purpose

Reverse letters or numbers in nucleotide sequence

Syntax

```
SeqR = seqreverse(SeqNT)
```

Arguments

SeqNT	Enter a nucleotide sequence. Enter either a character string with the characters `A`, `T` (`U`), `G`, `C`, and ambiguous characters `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, `V`, `N`, or a vector of integers. You can also enter a structure with the field `Sequence`.
SeqR	Returns a sequence in the same format as the nucleotide sequence. For example, if *SeqNT* is an integer sequence, then so is *SeqR*.

Description

`seqreverse` calculates the reverse strand of a DNA or RNA sequence.

`SeqR = seqreverse(SeqNT)` calculates the reverse strand 3' --> 5' of the nucleotide sequence.

Examples

Reverse a nucleotide sequence.

```
s = 'ATCG'
seqreverse(s)

ans =
GCTA
```

See Also

Bioinformatics Toolbox functions: `seqcomplement`, `seqrcomplement`, `seqtool`

MATLAB function: `fliplr`

seqshoworfs

Purpose

Display open reading frames in sequence

Syntax

```
seqshoworfs(SeqNT)
seqshoworfs(SeqNT, ...'Frames', FramesValue, ...)
seqshoworfs(SeqNT, ...'GeneticCode', GeneticCodeValue, ...)
seqshoworfs(SeqNT, ...'MinimumLength', MinimumLengthValue,
    ...)
seqshoworfs(SeqNT, ...'AlternativeStartCodons',
    AlternativeStartCodonsValue, ...)
seqshoworfs(SeqNT, ...'Color', ColorValue, ...)
seqshoworfs(SeqNT, ...'Columns', ColumnsValue, ...)
```

Arguments

SeqNT	Nucleotide sequence. Enter either a character string with the characters `A`, `T` (`U`), `G`, `C`, and ambiguous characters `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, `V`, `N`, or a vector of integers. You can also enter a structure with the field `Sequence`.
FramesValue	Property to select the frame. Enter `1`, `2`, `3`, `-1`, `-2`, `-3`, enter a vector with integers, or `'all'`. The default value is the vector `[1 2 3]`. Frames `-1`, `-2`, and `-3` correspond to the first, second, and third reading frames for the reverse complement.
GeneticCodeValue	Genetic code name. Enter a code number or a code name from the table see .
MinimumLengthValue	Property to set the minimum number of codons in an ORF.

AlternativeStartCodonsValue	Property to control using alternative start codons. Enter either `true` or `false`. The default value is `false`.
ColorValue	Property to select the color for highlighting the reading frame. Enter either a `1`-by-`3` RGB vector specifying the intensity (`0 to 255`) of the red, green, and blue components of the color, or a character from the following list: `'b'`—blue, `'g'`—green, `'r'`—red, `'c'`—cyan, `'m'`—magenta, or `'y'`—yellow. To specify different colors for the three reading frames, use a `1`-by-`3` cell array of color values. If you are displaying reverse complement reading frames, then COLOR should be a `1`-by-`6` cell array of color values.
ColumnsValue	Property to specify the number of columns in the output.

Description

`seqshoworfs` identifies and highlights all open reading frames using the standard or an alternative genetic code.

`seqshoworfs(`*`SeqNT`*`)` displays the sequence with all open reading frames highlighted, and it returns a structure of start and stop positions for each ORF in each reading frame. The standard genetic code is used with start codon `'AUG'` and stop codons `'UAA'`, `'UAG'`, and `'UGA'`.

`seqshoworfs(`*`SeqNT`*`, ...'`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `seqshoworfs` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`seqshoworfs(SeqNT, ...'Frames', FramesValue, ...)` specifies the reading frames to display. The default is to display the first, second, and third reading frames with ORFs highlighted in each frame.

`seqshoworfs(SeqNT, ...'GeneticCode', GeneticCodeValue, ...)` specifies the genetic code to use for finding open reading frames.

`seqshoworfs(SeqNT, ...'MinimumLength', MinimumLengthValue, ...)` sets the minimum number of codons for an ORF to be considered valid. The default value is `10`.

`seqshoworfs(SeqNT, ...'AlternativeStartCodons', AlternativeStartCodonsValue, ...)` uses alternative start codons if `AlternativeStartCodons` is set to `true`. For example, in the human mitochondrial genetic code, `AUA` and `AUU` are known to be alternative start codons. For more details on alternative start codons, see

```
http://www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=t#SG1
```

`seqshoworfs(SeqNT, ...'Color', ColorValue, ...)` selects the color used to highlight the open reading frames in the output display. The default color scheme is blue for the first reading frame, red for the second, and green for the third frame.

`seqshoworfs(SeqNT, ...'Columns', ColumnsValue, ...)` specifies how many columns per line to use in the output. The default value is `64`.

Examples

Look for the open reading frames in a random nucleotide sequence.

```
s = randseq(200, 'alphabet', 'dna');
seqshoworfs(s);
```


Open Reading Frames
Frame 1
000001
TAGCTTCATCGTTGACTTCTACTAAAAGCAAGCTCCTGAGTAGCTGGCCAAGCGAGCTTGCTTG
000065
TGCCCGGCTGCGGCGGTTGTATCCTGAATACGCCATGCGCCAGTGGACTGCGTAGACCTATTTT
000129
CCAGCTGCGCCTGATGAAGGCGCAACACGAAGGAAAGACGGGACCCAGGGCGACGTCCTATTAA
000193 AAGATAAT
Frame 2
000001
TAGCTTCATCGTTGACTTCTACTAAAAGCAAGCTCCTGAGTAGCTGGCCAAGCGAGCTTGCTTG
000065
TGCCCGGCTGCGGCGGTTGTATCCTGAATACGCCATGCGCCAGTGGACTGCGTAGACCTATTTT
000129
CCAGCTGCGCCTGATGAAGGCGCAACACGAAGGAAAGACGGGACCCAGGGCGACGTCCTATTAA
000193 AAGATAAT
Frame 3
000001
TAGCTTCATCGTTGACTTCTACTAAAAGCAAGCTCCTGAGTAGCTGGCCAAGCGAGCTTGCTTG
000065
TGCCCGGCTGCGGCGGTTGTATCCTGAATACGCCATGCGCCAGTGGACTGCGTAGACCTATTTT
000129
CCAGCTGCGCCTGATGAAGGCGCAACACGAAGGAAAGACGGGACCCAGGGCGACGTCCTATTAA
000193 AAGATAAT

Identify the open reading frames in a GenBank sequence.

```
HLA_DQB1 = getgenbank('NM_002123');
seqshoworfs(HLA_DQB1.Sequence);
```

See Also

Bioinformatics Toolbox functions: `codoncount`, `cpgisland`, `geneticcode`, `seqdisp`, `seqshowwords`, `seqtool`, `seqwordcount`

MATLAB function: `regexp`

Purpose

Graphically display words in sequence

Syntax

```
seqshowwords(Seq, Word)
seqshowwords(Seq, Word, ...'Color', ColorValue, ...)
seqshowwords(Seq, Word, ...'Columns', ColumnsValue, ...)
seqshowwords(Seq, Word, ...'Alphabet', AlphabetValue, ...)
```

Arguments

Seq	Enter either a nucleotide or amino acid sequence. You can also enter a structure with the field `Sequence`.
Word	Enter a short character sequence.
ColorValue	Property to select the color for highlighted characters. Enter a `1`-by-3 RGB vector specifying the intensity (`0 255`) of the red, green, and blue components, or enter a character from the following list: `'b'`– blue, `'g'`– green, `'r'`– red, `'c'`– cyan, `'m'`– magenta, or `'y'`– yellow. The default color is red `'r'`.
ColumnsValue	Property to specify the number of characters in a line. Default value is `64`.
AlphabetValue	Property to select the alphabet. Enter `'AA'` for amino acid sequences or `'NT'` for nucleotide sequences. The default is `'NT'`.

Description

`seqshowwords(`*`Seq`*`, `*`Word`*`)` displays the sequence with all occurrences of a word highlighted, and returns a structure with the start and stop positions for all occurrences of the word in the sequence.

`seqshowwords(`*`Seq`*`, `*`Word`*`, ...'`*`PropertyName`*`',` *`PropertyValue`*`, ...)` calls `seqshowwords` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`seqshowwords(`*`Seq`*`, `*`Word`*`, ...'Color', `*`ColorValue`*`, ...)` selects the color used to highlight the words in the output display.

`seqshowwords(`*`Seq`*`, `*`Word`*`, ...'Columns', `*`ColumnsValue`*`, ...)` specifies how many columns per line to use in the output.

`seqshowwords(`*`Seq`*`, `*`Word`*`, ...'Alphabet', `*`AlphabetValue`*`, ...)` selects the alphabet for the sequence (*`Seq`*) and the word (*`Word`*).

If the search work (*`Word`*) contains nucleotide or amino acid symbols that represent multiple possible symbols, then `seqshowwords` shows all matches. For example, the symbol `R` represents either `G` or `A` (purines). If *`Word`* is `'ART'`, then `seqshowwords` shows occurrences of both `'AAT'` and `'AGT'`.

Examples

This example shows two matches, `'TAGT'` and `'TAAT'`, for the word `'BART'`.

```
seqshowwords('GCTAGTAACGTATATATAAT','BART')

ans =
    Start: [3 17]
    Stop: [6 20]

000001 GCTAGTAACGTATATATAAT
```

`seqshowwords` does not highlight overlapping patterns multiple times. This example highlights two places, the first occurrence of `'TATA'` and the `'TATATATA'` immediately after `'CG'`. The final `'TA'` is not highlighted because the preceding `'TA'` is part of an already matched pattern.

```
seqshowwords('GCTATAACGTATATATATA','TATA')

ans =
    Start: [3 10 14]
```

```
    Stop: [6 13 17]

000001 GCTATAACGTATATATATA
```

To highlight all multiple repeats of TA, use the regular expression 'TA(TA)*TA'.

```
seqshowwords('GCTATAACGTATATATATA','TA(TA)*TA')

ans =
    Start: [3 10]
    Stop: [6 19]

000001 GCTATAACGTATATATATA
```

See Also

Bioinformatics Toolbox functions: palindromes, cleave, restrict, seqdisp, seqtool, seqwordcount

MATLAB functions: strfind, regexp

Purpose

Open tool to interactively explore biological sequences

Syntax

```
seqtool(Seq)
seqtool(..., 'PropertyName', PropertyValue,...)
seqtool(..., 'Alphabet', AlphabetValue)
```

Arguments

Seq	Struct with a field Sequence, a character array, or a file name with an extension of .gbk, .gpt, .fasta, .fa, or .ebi

Description

`seqtool(`*`Seq`*`)` loads a sequence (*Seq*) into the `seqtool` GUI.

`seqtool(..., '`*`PropertyName`*`', `*`PropertyValue`*`,...)` defines optional properties using property name/value pairs.

`seqtool(..., 'Alphabet', `*`AlphabetValue`*`)` specifies an alphabet (*AlphabetValue*) for the sequence (*Seq*). Default is `'AA'`, except when all of the symbols in the sequence are `A`, `C`, `G`, `T`, and `-`, then *AlphabetValue* is set to `'NT'`. Use `'AA'` when you want to force an amino acid sequence alphabet.

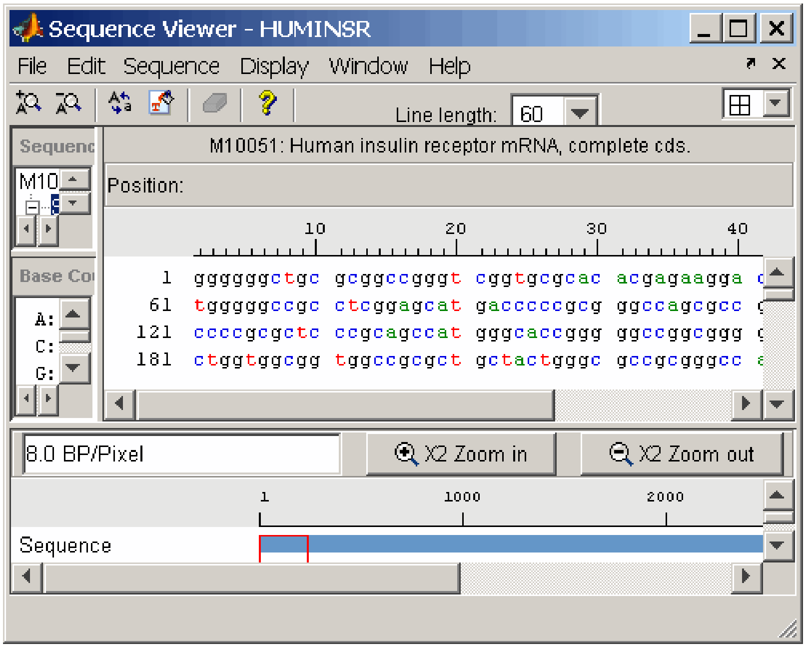
Example

1 Get a sequence from Genbank.

```
S = getgenbank('M10051')
```

2 Open the sequence tool window with the sequence.

```
seqtool(S)
```



See Also

Bioinformatics Toolbox functions: `aa2nt`, `aacount`, `aminolookup`, `basecount`, `baselookup`, `dimercount`, `emblread`, `fastaread`, `fastawrite`, `genbankread`, `geneticcode`, `genpeptread`, `getembl`, `getgenbank`, `getgenpept`, `nt2aa`, `proteinplot`, `seqcomplement`, `seqdisp`, `seqrcomplement`, `seqreverse`, `seqshoworfs`, `seqshowwords`, `seqwordcount`

seqwordcount

Purpose

Count number of occurrences of word in sequence

Syntax

```
seqwordcount(Seq, Word)
```

Arguments

`Seq`	Enter a nucleotide or amino acid sequence of characters. You can also enter a structure with the field `Sequence`.
`Word`	Enter a short sequence of characters.

Description

`seqwordcount(Seq, Word)` counts the number of times that a word appears in a sequence, and then returns the number of occurrences of that word.

If `Word` contains nucleotide or amino acid symbols that represent multiple possible symbols (ambiguous characters), then `seqwordcount` counts all matches. For example, the symbol `R` represents either `G` or `A` (purines). For another example, if `word` equals `'ART'`, then `seqwordcount` counts occurrences of both `'AAT'` and `'AGT'`.

Examples

`seqwordcount` does not count overlapping patterns multiple times. In the following example, `seqwordcount` reports three matches. `TATATATA` is counted as two distinct matches, not three overlapping occurrences.

```
seqwordcount('GCTATAACGTATATATAT','TATA')

ans =
      3
```

The following example reports two matches (`'TAGT'` and `'TAAT'`). `B` is the ambiguous code for `G`, `T`, or `C`, while `R` is an ambiguous code for `G` and `A`.

```
seqwordcount('GCTAGTAACGTATATATAAT','BART')

ans =
      2
```

See Also

Bioinformatics Toolbox functions `codoncount`, `seqshoworfs`, `seqshowwords`, `seqtool`, `seq2regexp`

MATLAB functions `strfind`

showalignment

Purpose

Sequence alignment with color

Syntax

```
showalignment(Alignment)
showalignment(Alignment, ...'MatchColor',
MatchColorValue, ...)
showalignment(Alignment,
...'SimilarColor' SimilarColorValue,
    ...)
showalignment(Alignment, ...'StartPointers',
    StartPointersValue, ...)
showalignment(Alignment, ...'Columns', ColumnsValue, ...)
```

Arguments

Alignment	For pairwise alignments, matches and similar residues are highlighted and *Alignment* is the output from one of the functions `nwalign` or `swalign`. For multiple sequence alignment highly conserved columns are highlighted and *Alignment* is the output from the function `multialign`.
MatchColorValue	Property to select the color to highlight matching characters. Enter a `1`-by-`N` RGB vector specifying the intensity (`0` to `255`) of the red, green, and blue components, or enter a character from the following list: `'b'`– blue, `'g'`– green, `'r'`– red, `'c'`– cyan, `'m'`– magenta, or `'y'`– yellow. The default color is red, `'r'`.
SimilarColorValue	Property to select the color to highlight similar characters. Enter a `1`-by-`3` RGB vector or color character. The default color is magenta.

StarterPointersValue	Property to specify the starting indices of the aligned sequences. `StartPointers` is the two element vector returned as the third output of the function `swalign`.
ColumnsValue	Property to specify the number of characters in a line. Enter the number of characters to display in one row. The default value is `64`.

Description

`showalignment(`*`Alignment`*`)` displays an alignment in a MATLAB figure window.

`showalignment(`*`Alignment`*`, ...'`*`PropertyName`*`',` *`PropertyValue`*`, ...)` calls `showalignment` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`showalignment(`*`Alignment`*`, ...'MatchColor',` *`MatchColorValue`*`, ...)` selects the color to highlight the matches in the output display. The default color is red. For example, to use cyan, enter `'c'` or `[0 255 255]`.

`showalignment(`*`Alignment`*`, ...'SimilarColor'` *`SimilarColorValue`*`, ...)` selects the color to highlight similar residues that are not exact matches. The default color is magenta.

The following options are only available when showing pairwise alignments:

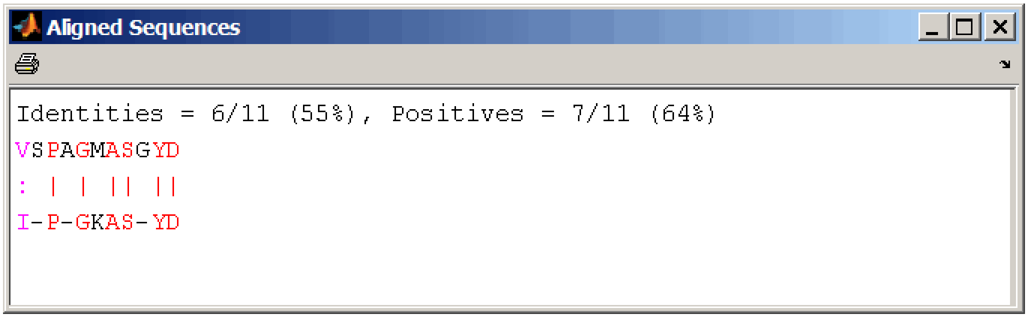
`showalignment(`*`Alignment`*`, ...'StartPointers',` *`StartPointersValue`*`, ...)` specifies the starting indices in the original sequences of a local alignment.

`showalignment(`*`Alignment`*`, ...'Columns',` *`ColumnsValue`*`, ...)` specifies how many columns per line to use in the output, and labels the start of each row with the sequence positions.

Examples

Enter two amino acid sequences and show their alignment.

```
[Score, Alignment] = nwalign('VSPAGMASGYD','IPGKASYD');
showalignment(Alignment);
```



Enter a multiply aligned set of sequences and show their alignment.

```
gag = multialignread('aagag.aln');
showalignment(gag)
```

See Also

Bioinformatics Toolbox functions: `nwalign`, `swalign`

Purpose

Plot Hidden Markov Model (HMM) profile

Syntax

```
showhmmprof(Model)
showhmmprof(..., 'PropertyName', PropertyValue,...)
showhmmprof(..., 'Scale', ScaleValue)
showhmmprof(..., 'Order', OrderValue)
```

Arguments

Model	Hidden Markov model created by the function `gethmmprof` or `pfamhmmread`.
ScaleValue	Property to select a probability scale. Enter one of the following values: • `'logprob'` — Log probabilities • `'prob'` — Probabilities • `'logodds'` — Log-odd ratios
OrderValue	Property to specify the order of the amino acid alphabet. Enter a character string with the 20 standard amino acids characters `A R N D C Q E G H I L K M F P S T W Y V`. The ambiguous characters `B Z X` are not allowed.

Description

`showhmmprof(`*`Model`*`)` plots a profile hidden Markov model described by the structure *`Model`*.

`showhmmprof(..., '`*`PropertyName`*`',` *`PropertyValue`*`,...)` defines optional properties using property name/value pairs.

`showhmmprof(..., 'Scale',` *`ScaleValue`*`)` specifies the scale to use. If log probabilities (*`ScaleValue`*`='logprob'`), probabilities (*`ScaleValue`*`='prob'`), or log-odd ratios (*`ScaleValue`*`='logodds'`). To compute the log-odd ratios, the null model probabilities are used for symbol emission and equally distributed transitions are used for the null transition probabilities. The default *`ScaleValue`* is `'logprob'`.

`showhmmprof(..., 'Order',` *`OrderValue`*`)` specifies the order in which the symbols are arranged along the vertical axis. This option allows you reorder the alphabet and group the symbols according to their properties.

Examples

1 Load a model example.

```
model = pfamhmmread('pf00002.ls')
```

2 Plot the profile.

```
showhmmprof(model, 'Scale', 'logodds')
```

3 Order the alphabet by hydrophobicity.

```
hydrophobic = 'IVLFCMAGTSWYPHNDQEKR'
```

4 Plot the profile.

```
showhmmprof(model, 'Order', hydrophobic)
```

See Also

Bioinformatics Toolbox functions: `gethmmprof`, `hmmprofalign`, `hmmprofestimate`, `hmmprofgenerate`, `hmmprofstruct`, `pfamhmmread`

Purpose

Read data from SPOT file

Syntax

```
SPOTData = sptread(File)
SPOTData = sptread(File, 'CleanColNames',
CleanColNamesValue)
```

Arguments

File	Either of the following: • String specifying a file name, a path and file name, or a URL pointing to a file. The referenced file is a SPOT-formatted file (ASCII text file). If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Directory. • MATLAB character array that contains the text of a SPOT-formatted file.
CleanColNamesValue	Property to control using valid MATLAB variable names.

Description

SPOTData = sptread(*File*) reads a SPOT formatted file, *File*,) and creates a MATLAB structure, *SPOTData*, containing the following fields:

```
Header
Data
Blocks
Columns
Rows
IDs
ColumnNames
Indices
Shape
```

`SPOTData = sptread(File, 'CleanColNames', CleanColNamesValue)` The column names in the SPOT file contain periods and some characters that cannot be used in MATLAB variable names. If you plan to use the column names as variable names in a function, use this option with `CleanColNames` set to `true` and the function will return the field `ColumnNames` with valid variable names.

The `Indices` field of the structure includes the MATLAB indices that you can use for plotting heat maps of the data.

Examples

1. Read in a sample SPOT file and plot the median foreground intensity for the 635 nm channel. Note that the example file `spotdata.txt` is not provided with Bioinformatics Toolbox.

```
spotStruct = sptread('spotdata.txt')
maimage(spotStruct,'Rmedian');
```

2. Alternatively, create a similar plot using more basic graphics commands.

```
Rmedian = magetfield(spotStruct,'Rmedian');
imagesc(Rmedian(spotStruct.Indices));
colormap bone
colorbar
```

See Also

Bioinformatics Toolbox functions: `affyread`, `agferead`, `celintensityread`, `geosoftread`, `gprread`, `imageneread`, `maboxplot`, `magetfield`

Purpose

Classify data using support vector machine

Syntax

```
Group = svmclassify(SVMStruct, Sample)
Group = svmclassify(SVMStruct, Sample, 'Showplot',
ShowplotValue)
```

Description

`Group = svmclassify(SVMStruct, Sample)` classifies each row of the data in `Sample` using the information in a support vector machine classifier structure `SVMStruct`, created using the `svmtrain` function. `Sample` must have the same number of columns as the data used to train the classifier in `svmtrain`. `Group` indicates the group to which each row of `Sample` has been assigned.

`Group = svmclassify(SVMStruct, Sample, 'Showplot', ShowplotValue)` controls the plotting of the sample data in the figure created using the `Showplot` property with the `svmtrain` function.

Examples

1. Load the sample data, which includes Fisher's iris data of 5 measurements on a sample of 150 irises.

```
load fisheriris
```

2. Create `data`, a two-column matrix containing sepal length and sepal width measurements for 150 irises.

```
data = [meas(:,1), meas(:,2)];
```

3. From the `species` vector, create a new column vector, `groups`, to classify data into two groups: Setosa and non-Setosa.

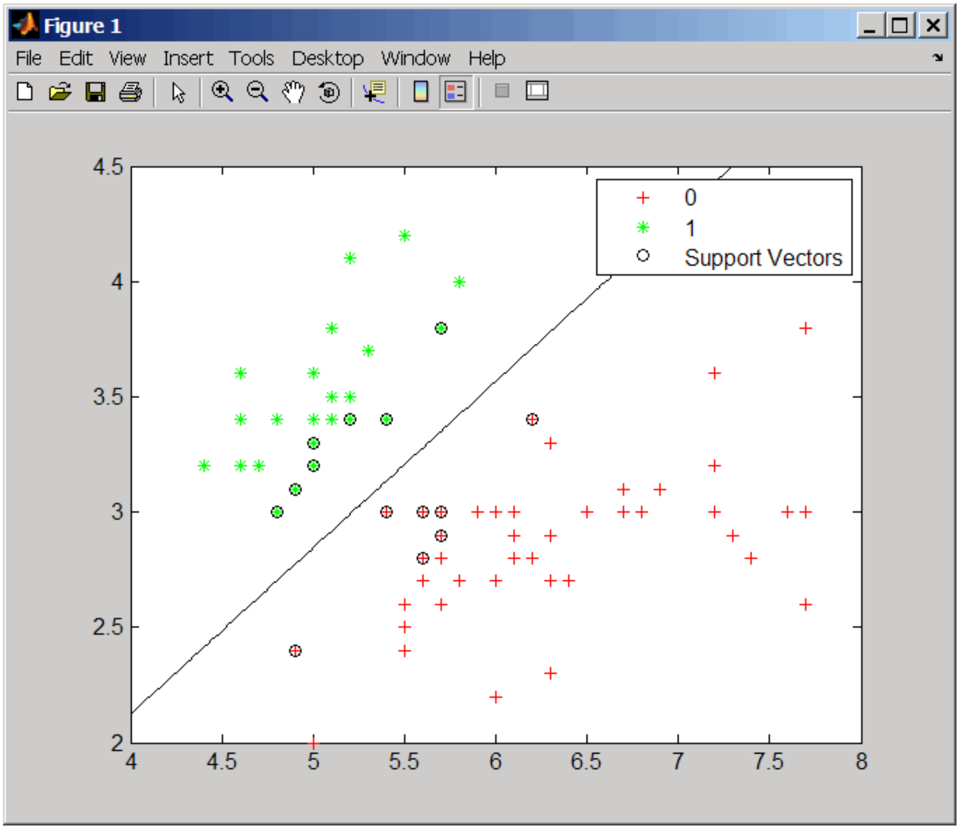
```
groups = ismember(species,'setosa');
```

4. Randomly select training and test sets.

```
[train, test] = crossvalind('holdOut',groups);
cp = classperf(groups);
```

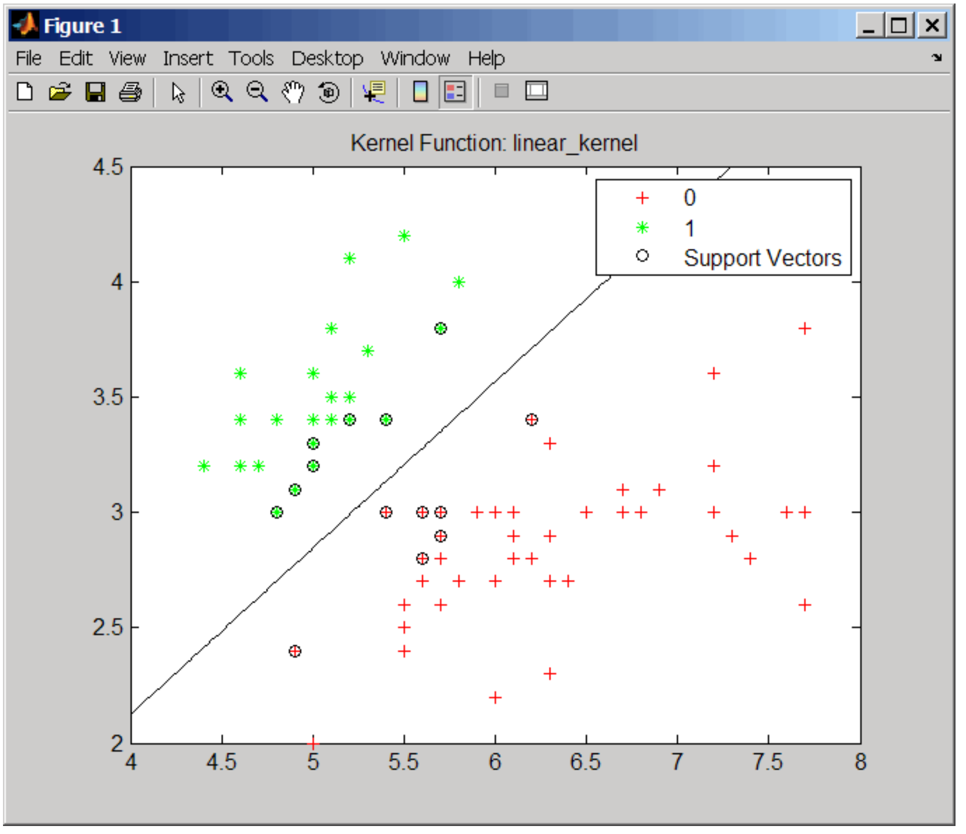
5 Use the svmtrain function to train an SVM classifier using a linear kernel function and plot the grouped data.

```
svmStruct = svmtrain(data(train,:),groups(train),'showplot',true);
```



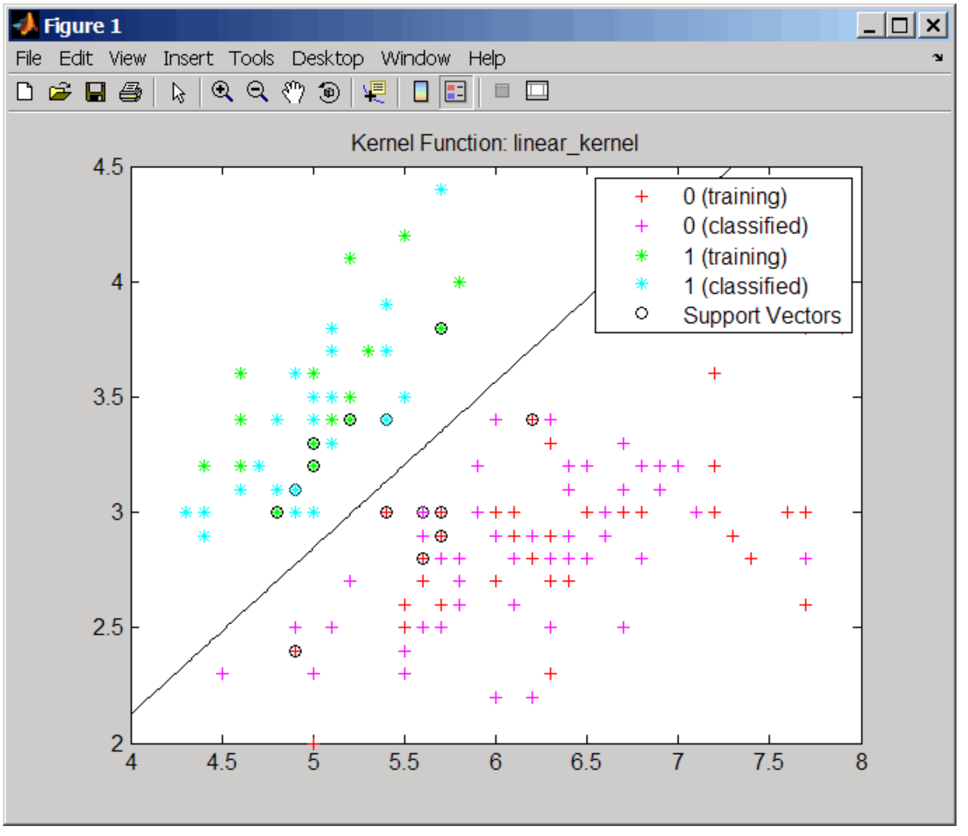
6 Add a title to the plot, using the KernelFunction field from the svmStruct structure as the title.

```
title(sprintf('Kernel Function: %s',...
              func2str(svmStruct.KernelFunction)),...
              'interpreter','none');
```



7 Classify the test set using a support vector machine.

```
classes = svmclassify(svmStruct,data(test,:),'showplot',true);
```

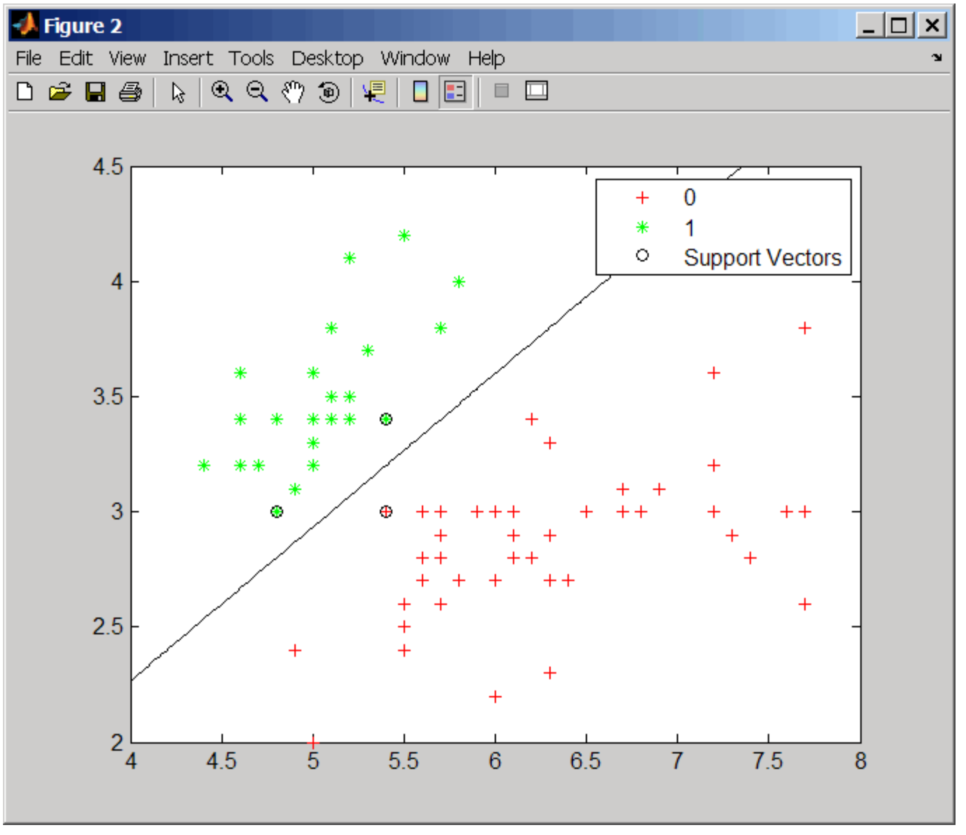


8 Evaluate the performance of the classifier.

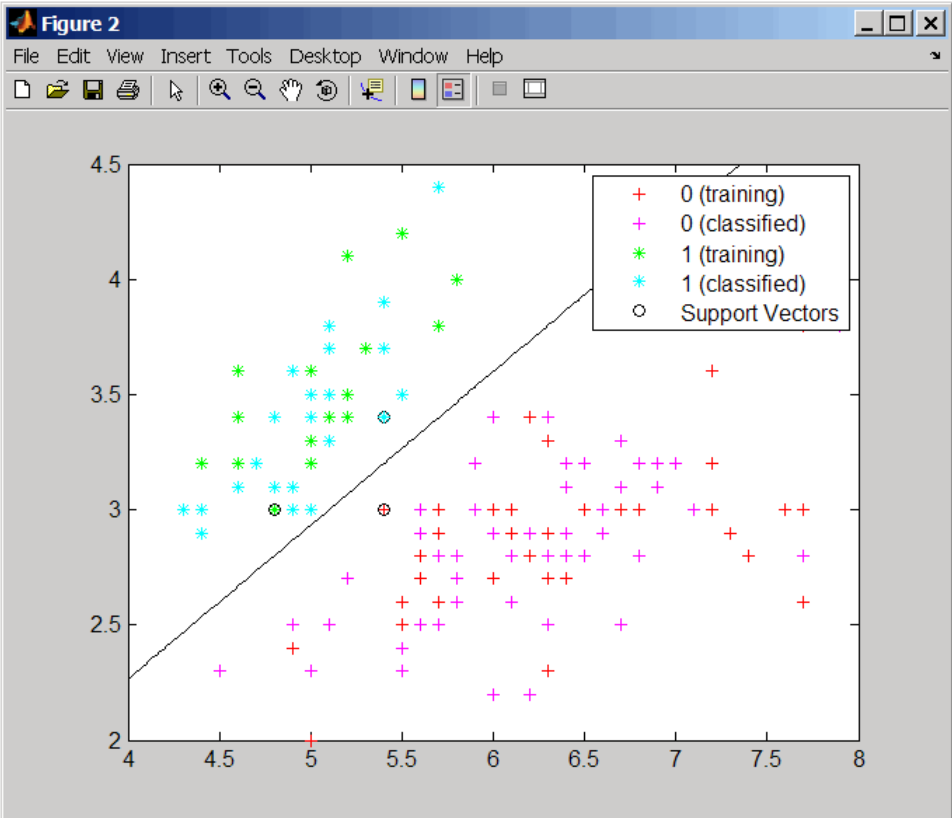
```
classperf(cp,classes,test);
cp.CorrectRate

ans =

    0.9867
```

9 Use a one-norm, hard margin support vector machine classifier by changing the `boxconstraint` property.

```
figure
svmStruct = svmtrain(data(train,:),groups(train),...
                     'showplot',true,'boxconstraint',1e6);
```




```
classes = svmclassify(svmStruct,data(test,:),'showplot',true);
```



10 Evaluate the performance of the classifier.

```
classperf(cp,classes,test);
cp.CorrectRate

ans =

    0.9867
```

References

[1] Kecman, V., Learning and Soft Computing, MIT Press, Cambridge, MA. 2001.

[2] Suykens, J.A.K., Van Gestel, T., De Brabanter, J., De Moor, B., and Vandewalle, J., Least Squares Support Vector Machines, World Scientific, Singapore, 2002.

[3] Scholkopf, B., and Smola, A.J., Learning with Kernels, MIT Press, Cambridge, MA. 2002.

[4] Cristianini, N., and Shawe-Taylor, J. (2000). An Introduction to Support Vector Machines and Other Kernel-based Learning Methods, First Edition (Cambridge: Cambridge University Press). `http://www.support-vector.net/`

See Also

Bioinformatics Toolbox functions: `classperf`, `crossvalind`, `knnclassify`, `svmtrain`

Statistics Toolbox function: `classify`

Optimization Toolbox function: `quadprog`

Purpose

Create or edit Sequential Minimal Optimization (SMO) options structure

Syntax

```
SMO_OptsStruct = svmsmoset('Property1Name', Property1Value,
   'Property2Name', Property2Value, ...)
SMO_OptsStruct = svmsmoset(OldOpts, 'Property1Name',
   Property1Value, 'Property2Name', Property2Value, ...)
SMO_OptsStruct = svmsmoset(OldOpts, NewOpts)
```

Arguments

OldOpts	Structure that specifies options used by the SMO method used by the svmtrain function.
NewOpts	Structure that specifies options used by the SMO method used by the svmtrain function.

PropertyName	Description of *PropertyValue*
TolKKT	Value that specifies the tolerance with which the KKT conditions are checked. KKT conditions are Karush-Kuhn-Tucker conditions. Default is 1.0000e-003.
MaxIter	Integer that specifies the maximum number of iterations of the main loop. If this limit is exceeded before the algorithm converges, then the algorithm stops and returns an error. Default is 1500.

PropertyName	**Description of *PropertyValue***
Display	String that specifies the level of information about the optimization iterations that is displayed as the algorithm runs. Choices are: • off — Default. Reports nothing. • iter — Reports every 10 iterations. • final — Reports only when the algorithm finishes.
KKTViolationLevel	Value that specifies the fraction of variables allowed to violate the KKT conditions. Choices are any value ≥ 0 and < 1. Default is 0. For example, if you set KKTViolationLevel to 0.05, then 5% of the variables are allowed to violate the KKT conditions. **Tip** Set this option to a positive value to help the algorithm converge if it is fluctuating near a good solution. For more information on KKT conditions, see Cristianini, et al. 2000.
KernelCacheLimit	Value that specifies the size of the kernel matrix cache. The algorithm keeps a matrix with up to KernelCacheLimit × KernelCacheLimit double-precision, floating-point numbers in memory. Default is 7500.

Return Values

SMO_OptsStruct Structure that specifies options used by the SMO method used by the svmtrain function.

svmsmoset

Description

SMO_OptsStruct = svmsmoset('*Property1Name*', *Property1Value*, '*Property2Name*', *Property2Value*, ...) creates *SMO_OptsStruct*, an SMO options structure from the specified inputs. This structure can be used as input for the svmtrain function.

SMO_OptsStruct = svmsmoset(*OldOpts*, '*Property1Name*', *Property1Value*, '*Property2Name*', *Property2Value*, ...) alters the options in *OldOpts*, an existing SMO options structure, with the specified inputs, creating a new output options structure.

SMO_OptsStruct = svmsmoset(*OldOpts*, *NewOpts*) alters the options in *OldOpts*, an existing SMO options structure, with the options specified in *NewOpts*, another SMO options structure, creating a new output options structure.

Examples

1 Create an SMO options structure and specify the Display, MaxIter, and KernelCacheLimit properties.

```
opts = svmsmoset('Display','final','MaxIter',200,...
                 'KernelCacheLimit',1000)

opts =

              Display: 'final'
               TolKKT: 1.0000e-003
              MaxIter: 200
    KKTViolationLevel: 0
     KernelCacheLimit: 1000
```

2 Create an alternate SMO options structure from the previous structure. Specify different Display and KKTViolationLevel properties.

```
alt_opts = svmsmoset(opts,'Display','iter','KKTViolationLevel',.05)

alt_opts =

              Display: 'iter'
```

```
           TolKKT: 1.0000e-003
          MaxIter: 200
KKTViolationLevel: 0.0500
 KernelCacheLimit: 1000
```

References

[1] Cristianini, N., and Shawe-Taylor, J. (2000). An Introduction to Support Vector Machines and Other Kernel-based Learning Methods, First Edition (Cambridge: Cambridge University Press). `http://www.support-vector.net/`

[2] Platt, J.C. (1999). Sequential Minimal Optimization: A Fast Algorithm for Training Support Vector Machines. In Advances in Kernel Methods - Support Vector Learning, B. Scholkopf, J.C. Burges, and A.J. Smola, eds. (Cambridge MA: MIT Press), pp. 185–208.

See Also

Bioinformatics Toolbox functions: `svmclassify`, `svmtrain`

Optimization Toolbox functions: `optimset`

svmtrain

Purpose

Train support vector machine classifier

Syntax

```
SVMStruct = svmtrain(Training, Group)
SVMStruct = svmtrain(..., 'Kernel_Function',
Kernel_FunctionValue, ...)
SVMStruct = svmtrain(..., 'RBF_Sigma', RBFSigmaValue, ...)
SVMStruct = svmtrain(..., 'Polyorder', PolyorderValue, ...)
SVMStruct = svmtrain(..., 'Mlp_Params',
Mlp_ParamsValue, ...)
SVMStruct = svmtrain(..., 'Method', MethodValue, ...)
SVMStruct = svmtrain(..., 'QuadProg_Opts',
   QuadProg_OptsValue, ...)
SVMStruct = svmtrain(..., 'SMO_Opts', SMO_OptsValue, ...)
SVMStruct = svmtrain(..., 'BoxConstraint',
   BoxConstraintValue, ...)
SVMStruct = svmtrain(..., 'Autoscale', AutoscaleValue, ...)
SVMStruct = svmtrain(..., 'Showplot', ShowplotValue, ...)
```

Arguments

Training	Matrix of training data, where each row corresponds to an observation or replicate, and each column corresponds to a feature or variable.
Group	Column vector, character array, or cell array of strings for classifying data in *Training* into two groups. It has the same number of elements as there are rows in *Training*. Each element specifies the group to which the corresponding row in *Training* belongs.

Kernel_FunctionValue	String or function handle specifying the kernel function that maps the training data into kernel space. Choices are: • `linear` — Default. Linear kernel or dot product. • `quadratic` — Quadratic kernel. • `rbf` — Gaussian Radial Basis Function kernel with a default scaling factor, sigma, of `1`. • `polynomial` — Polynomial kernel with a default order of `3`. • `mlp` — Multilayer Perceptron kernel with default scale and bias parameters of `[1, -1]`. • `@functionname` — Handle to a kernel function specified using `@`and the `functionname`. For example, `@kfun`, or an anonymous function.
RBFSigmaValue	Positive number that specifies the scaling factor, sigma, in the radial basis function kernel. Default is `1`.
PolyorderValue	Positive number that specifies the order of a polynomial kernel. Default is `3`.
Mlp_ParamsValue	Two-element vector, `[p1, p2]`, that specifies the scale and bias parameters of the multilayer perceptron (mlp) kernel. `K = tanh(p1*U*V' + p2)`. `p1` must be `> 0`, and `p2` must be `< 0`. Default is `[1, -1]`.

MethodValue	String specifying the method to find the separating hyperplane. Choices are: • `QP` — Quadratic Programming (requires Optimization Toolbox). The classifier is a two-norm, soft-margin support vector machine. • `SMO` — Sequential Minimal Optimization. The classifier is a one-norm, soft-margin support vector machine. • `LS` — Least-Squares. If you installed Optimization Toolbox, the `QP` method is the default. Otherwise, the `SMO` method is the default.
QuadProg_OptsValue	An options structure created by the `optimset` function (Optimization Toolbox). This structure specifies options used by the `QP` method. For more information on creating this structure, see the `optimset` and `quadprog` reference pages.
SMO_OptsValue	An options structure created by the `svmsmoset` function. This structure specifies options used by the `SMO` method. For more information on creating this structure, see the `svmsmoset` function.

BoxConstraintValue	Box constraints for the soft margin. Choices are: • Strictly positive numeric scalar. • Array of strictly positive values with the number of elements equal to the number of rows in the *Training* matrix. If *BoxConstraintValue* is a scalar, it is automatically rescaled by N/(2*N1) for the data points of group one and by N/(2*N2) for the data points of group two. N1 is the number of elements in group one, N2 is the number of elements in group two, and N = N1 + N2. This rescaling is done to take into account unbalanced groups, that is cases where N1 and N2 have very different values. If *BoxConstraintValue* is an array, then each array element is taken as a box constraint for the data point with the same index. Default is a scalar value of `1`.
AutoscaleValue	Controls the shifting and scaling of data points before training. When *AutoscaleValue* is `true`, the columns of the input data matrix *Training* are shifted to zero mean and scaled to unit variance. Default is `false`.
ShowplotValue	Controls the display of a plot of the grouped data, including the separating line for the classifier, when using two-dimensional data. Choices are `true` or `false` (default).

Return Values

SVMStruct	Structure containing information about the trained SVM classifier, including the following fields: • `SupportVectors` • `Alpha` • `Bias` • `KernelFunction` • `KernelFunctionArgs` • `GroupNames` • `SupportVectorIndices` • `ScaleData` • `FigureHandles` **Tip** You can use *SVMStruct* as input to the `svmclassify` function, to use for classification.

Description

SVMStruct = `svmtrain(`*Training*, *Group*`)` trains a support vector machine (SVM) classifier using *Training*, a matrix of training data taken from two groups, specified by *Group*. `svmtrain` treats NaNs or empty strings in *Group* as missing values and ignores the corresponding rows of *Training*. Information about the trained SVM classifier is returned in *SVMStruct*, a structure with the following fields.

- `SupportVectors`
- `Alpha`
- `Bias`
- `KernelFunction`

- `KernelFunctionArgs`
- `GroupNames`
- `SupportVectorIndices`
- `ScaleData`
- `FigureHandles`

`SVMStruct` `= svmtrain(`*`Training`*`,` *`Group`*`, ...'`*`PropertyName`*`',` *`PropertyValue`*`, ...)` calls `svmtrain` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`SVMStruct` `= svmtrain(..., 'Kernel_Function',` *`Kernel_FunctionValue`*`, ...)` specifies the kernel function (*`Kernel_FunctionValue`*) that maps the training data into kernel space. *`Kernel_FunctionValue`* can be one of the following strings or a function handle:

- `linear` — Default. Linear kernel or dot product.
- `quadratic` — Quadratic kernel.
- `rbf` — Gaussian Radial Basis Function kernel with a default scaling factor, sigma, of `1`.
- `polynomial` — Polynomial kernel with a default order of `3`.
- `mlp` — Multilayer Perceptron kernel with default scale and bias parameters of `[1, -1]`.
- `@functionname` — Handle to a kernel function specified using `@`and the `functionname`. For example, `@kfun`, or an anonymous function.

A kernel function must be of the following form:

```
function K = kfun(U, V)
```

Input arguments U and V are matrices with m and n rows respectively. Return value K is an m-by-n matrix. If kfun is parameterized, you can use anonymous functions to capture the problem-dependent parameters. For example, suppose that your kernel function is:

```
function K = kfun(U,V,P1,P2)
K = tanh(P1*(U*V')+P2);
```

You can set values for P1 and P2 and then use an anonymous function as follows:

```
@(U,V) kfun(U,V,P1,P2)
```

For more information on the types of functions that can be used as kernel functions, see Cristianini and Shawe-Taylor, 2000.

SVMStruct = svmtrain(..., 'RBF_Sigma', *RBFSigmaValue*, ...) specifies the scaling factor, sigma, in the radial basis function kernel. *RBFSigmaValue* must be a positive number. Default is 1.

SVMStruct = svmtrain(..., 'Polyorder', *PolyorderValue*, ...) specifies the order of a polynomial kernel. *PolyorderValue* must be a positive number. Default is 3.

SVMStruct = svmtrain(..., 'Mlp_Params', *Mlp_ParamsValue*, ...) specifies the scale and bias parameters of the multilayer perceptron (mlp) kernel as a two-element vector, [p1, p2]. K = tanh(p1*U*V' + p2), p1 > 0, and p2 < 0. p1 must be > 0, and p2 must be < 0. Default is [1, -1].

SVMStruct = svmtrain(..., 'Method', *MethodValue*, ...) specifies the method to find the separating hyperplane. Choices are:

- QP — Quadratic Programming (requires Optimization Toolbox). The classifier is a two-norm, soft-margin support vector machine.
- SMO — Sequential Minimal Optimization. The classifier is a one-norm, soft-margin support vector machine.
- LS — Least-Squares.

If you installed Optimization Toolbox, the QP method is the default. Otherwise, the SMO method is the default.

Note If you specify the QP method, the classifier is a two-norm, soft-margin support vector machine.

SVMStruct = svmtrain(..., 'QuadProg_Opts', *QuadProg_OptsValue*, ...) specifies an options structure created by the optimset function (Optimization Toolbox). This structure specifies options used by the QP method. For more information on creating this structure, see the optimset and quadprog functions.

SVMStruct = svmtrain(..., 'SMO_Opts', *SMO_OptsValue*, ...) specifies an options structure created by svmsmoset function. This structure specifies options used by the SMO method. For more information on creating this structure, see the svmsmoset function.

SVMStruct = svmtrain(..., 'BoxConstraint', *BoxConstraintValue*, ...) specifies box constraints for the soft margin. *BoxConstraintValue* can be either of the following:

- Strictly positive numeric scalar
- Array of strictly positive values with the number of elements equal to the number of rows in the *Training* matrix

If *BoxConstraintValue* is a scalar, it is automatically rescaled by N/(2*N1) for the data points of group one and by N/(2*N2) for the data points of group two. N1 is the number of elements in group one, N2 is the number of elements in group two, and N = N1 + N2. This rescaling is done to take into account unbalanced groups, that is cases where N1 and N2 have very different values.

If *BoxConstraintValue* is an array, then each array element is taken as a box constraint for the data point with the same index.

Default is a scalar value of 1.

SVMStruct = svmtrain(..., 'Autoscale', *AutoscaleValue*, ...) controls the shifting and scaling of data points before training. When *AutoscaleValue* is true, the columns of the input data matrix *Training* are shifted to zero mean and scaled to unit variance. Default is false.

SVMStruct = svmtrain(..., 'Showplot', *ShowplotValue*, ...), controls the display of a plot of the grouped data , including the separating line for the classifier, when using two-dimensional data. Choices are true or false (default).

Memory Usage and Out of Memory Error

When you set 'Method' to 'QP', the svmtrain function operates on a data set containing N elements, it creates an (N+1)-by-(N+1) matrix to find the separating hyperplane. This matrix needs at least 8*(n+1)^2 bytes of contiguous memory. If this size of contiguous memory is not available, MATLAB displays an "out of memory" message.

When you set 'Method' to 'SMO', memory consumption is controlled by the SMO option KernelCacheLimit. For more information on the KernelCacheLimit option, see the svmsmoset function. The SMO algorithm stores only a submatrix of the kernel matrix, limited by the size specified by the KernelCacheLimit option. However, if the number of data points exceeds the size specified by the KernelCacheLimit option, the SMO algorithm slows down because it has to recalculate the kernel matrix elements.

When using svmtrain on large data sets, and you run out of memory or the optimization step is very time consuming, try either of the following:

- Use a smaller number of samples and use cross validation to test the performance of the classifier.
- Set 'Method' to 'SMO', and set the KernelCacheLimit option as large as your system permits. For information on setting the KernelCacheLimit option, see the svmsmoset function.

Tip If you set `'Method'` to `'SMO'`, setting the `'BoxConstraint'` property as small as possible will help the SMO algorithm run faster.

Examples

1. Load the sample data, which includes Fisher's iris data of 5 measurements on a sample of 150 irises.

```
load fisheriris
```

2. Create `data`, a two-column matrix containing sepal length and sepal width measurements for 150 irises.

```
data = [meas(:,1), meas(:,2)];
```

3. From the `species` vector, create a new column vector, `groups`, to classify data into two groups: Setosa and non-Setosa.

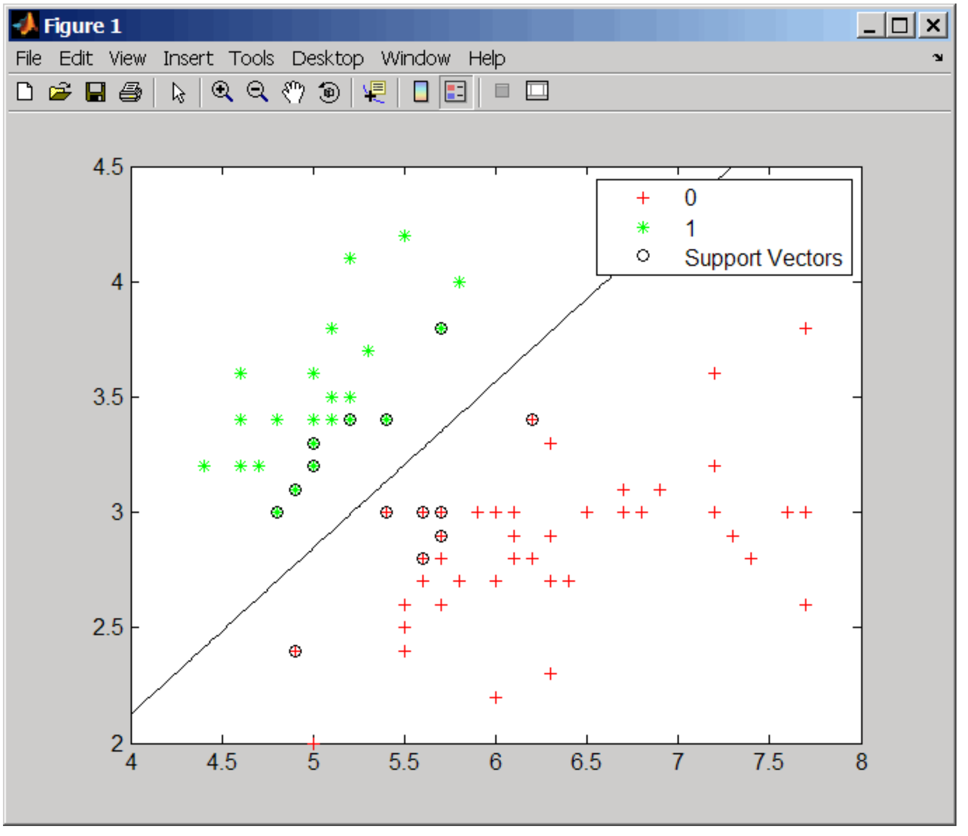
```
groups = ismember(species,'setosa');
```

4. Randomly select training and test sets.

```
[train, test] = crossvalind('holdOut',groups);
cp = classperf(groups);
```

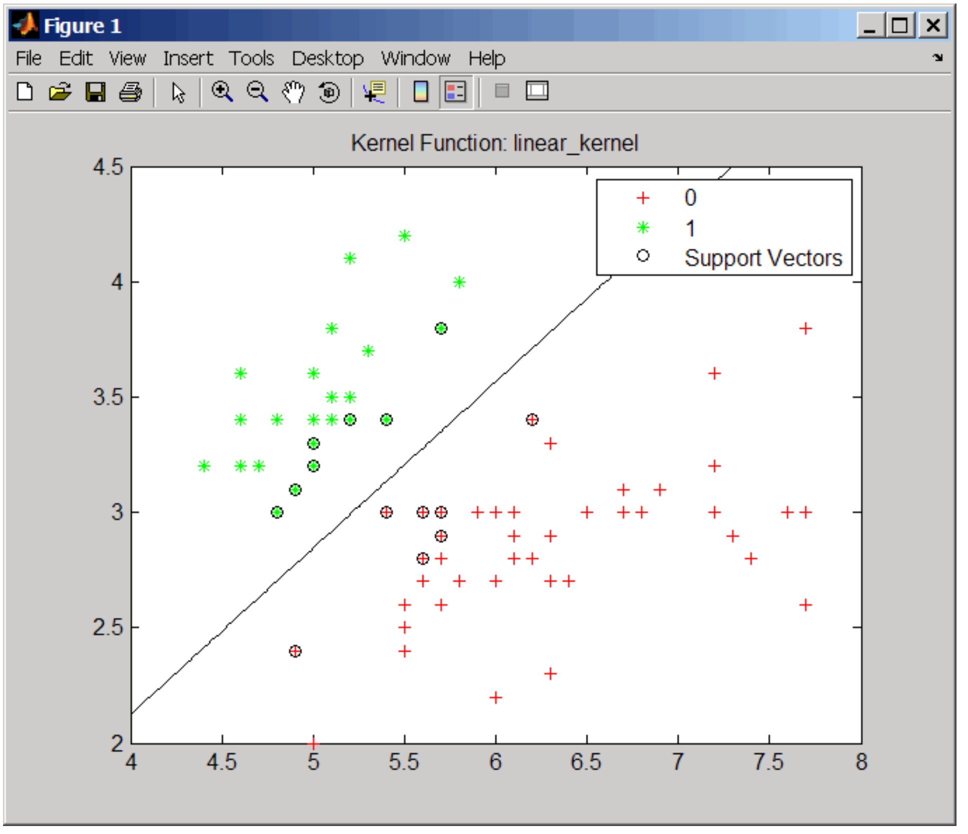
5. Train an SVM classifier using a linear kernel function and plot the grouped data.

```
svmStruct = svmtrain(data(train,:),groups(train),'showplot',true);
```



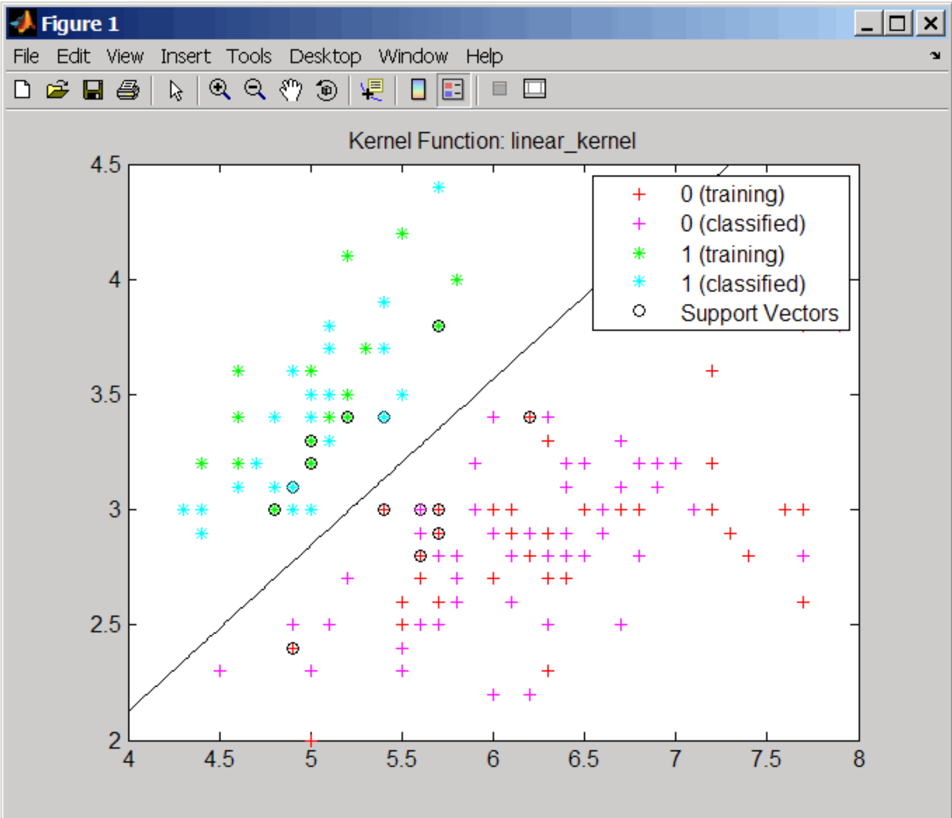
6 Add a title to the plot, using the `KernelFunction` field from the `svmStruct` structure as the title.

```
title(sprintf('Kernel Function: %s',...
             func2str(svmStruct.KernelFunction)),...
             'interpreter','none');
```



7 Use the `svmclassify` function to classify the test set.

```
classes = svmclassify(svmStruct,data(test,:),'showplot',true);
```

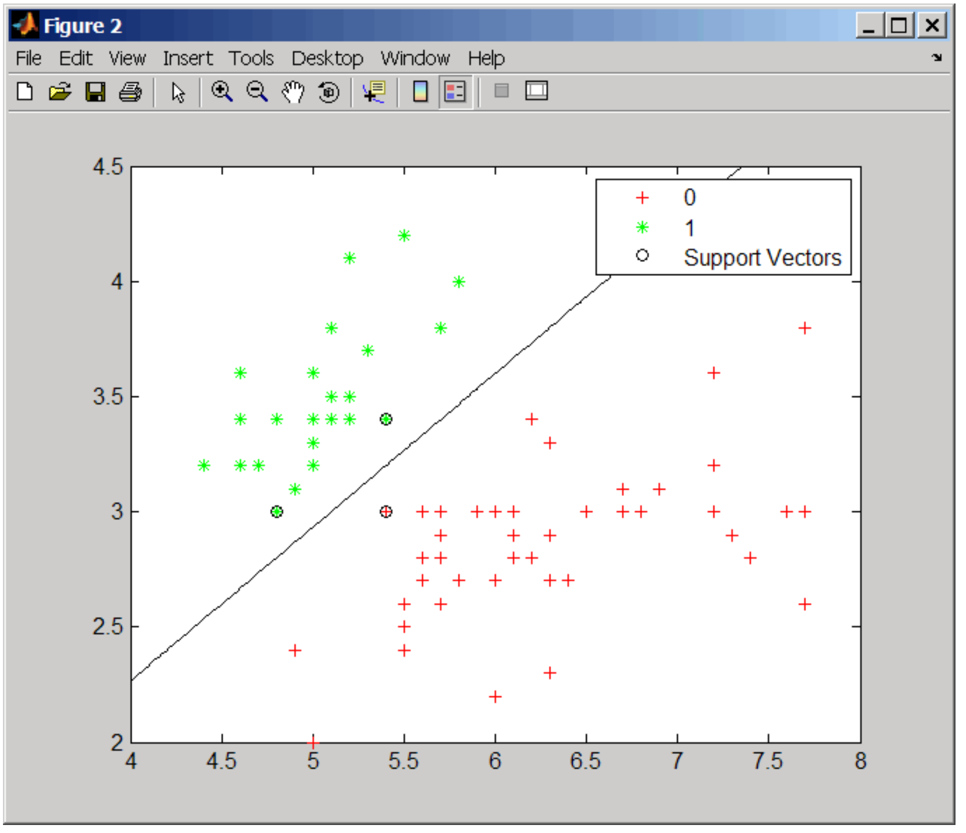


8 Evaluate the performance of the classifier.

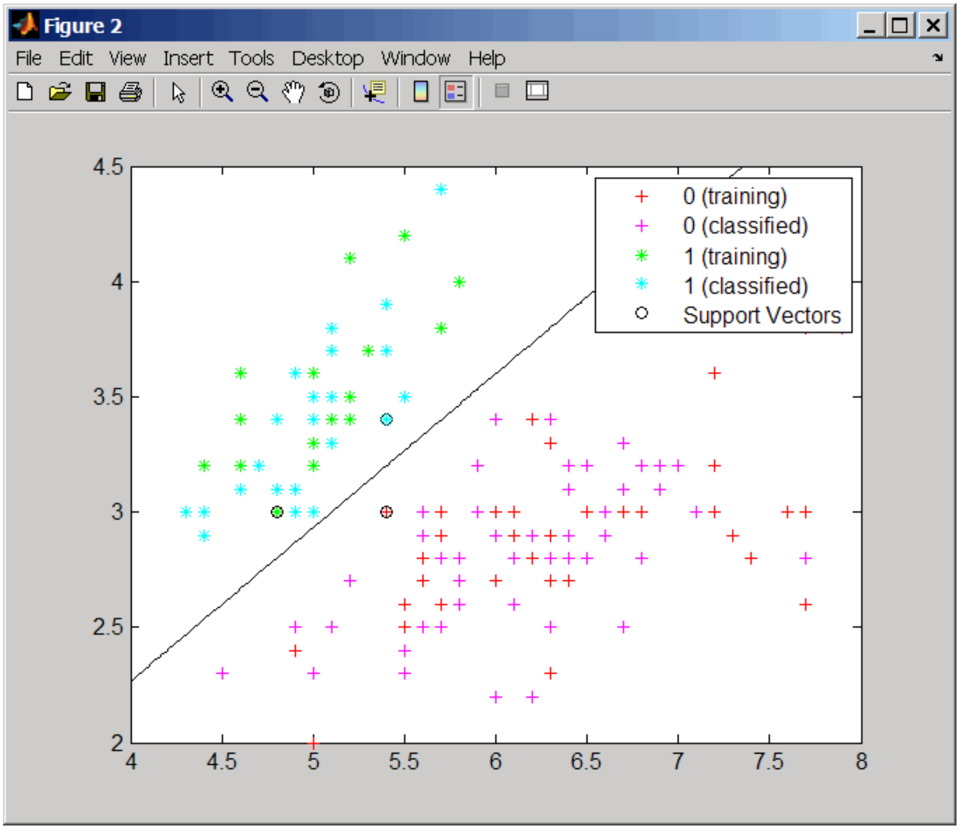
```
classperf(cp,classes,test);
cp.CorrectRate

ans =

     0.9867
```

9 Use a one-norm, hard margin support vector machine classifier by changing the `boxconstraint` property.

```
figure
svmStruct = svmtrain(data(train,:),groups(train),...
                     'showplot',true,'boxconstraint',1e6);
```




```
classes = svmclassify(svmStruct,data(test,:),'showplot',true);
```



10 Evaluate the performance of the classifier.

```
classperf(cp,classes,test);
cp.CorrectRate

ans =

    0.9867
```

References

[1] Kecman, V. (2001). Learning and Soft Computing (Cambridge, MA: MIT Press).

[2] Suykens, J.A.K., Van Gestel, T., De Brabanter, J., De Moor, B., and Vandewalle, J. (2002). Least Squares Support Vector Machines (Singapore: World Scientific).

[3] Scholkopf, B., and Smola, A.J. (2002). Learning with Kernels (Cambridge, MA: MIT Press).

[4] Cristianini, N. and Shawe-Taylor, J. (2000). An Introduction to Support Vector Machines and Other Kernel-based Learning Methods, First Edition (Cambridge: Cambridge University Press). `http://www.support-vector.net/`

See Also

Bioinformatics Toolbox functions: `knnclassify`, `svmclassify`, `svmsmoset`

Statistics Toolbox function: `classify`

Optimization Toolbox function: `quadprog`

MATLAB function: `optimset`

swalign

Purpose

Locally align two sequences using Smith-Waterman algorithm

Syntax

```
Score = swalign(Seq1, Seq2)
[Score, Alignment] = swalign(Seq1, Seq2)
[Score, Alignment, Start] = swalign(Seq1, Seq2)
... = swalign(Seq1,Seq2, ...'Alphabet', AlphabetValue)
... = swalign(Seq1,Seq2, ...'ScoringMatrix',
   ScoringMatrixValue, ...)
... = swalign(Seq1,Seq2, ...'Scale', ScaleValue, ...)
... = swalign(Seq1,Seq2, ...'GapOpen', GapOpenValue, ...)
... = swalign(Seq1,Seq2, ...'ExtendGap',
ExtendGapValue, ...)
... = swalign(Seq1,Seq2, ...'Showscore',
ShowscoreValue, ...)
```

Arguments

Seq1, *Seq2*

Amino acid or nucleotide sequences. Enter any of the following:

- Character string of letters representing amino acids or nucleotides, such as returned by `int2aa` or `int2nt`
- Vector of integers representing amino acids or nucleotides, such as returned by `aa2int` or `nt2int`
- Structure containing a `Sequence` field

Tip For help with letter and integer representations of amino acids and nucleotides, see Amino Acid Lookup Table on page 2-42 or Nucleotide Lookup Table on page 2-52.

AlphabetValue

String specifying the type of sequence. Choices are `'AA'` (default) or `'NT'`.

ScoringMatrixValue String specifying the scoring matrix to use for the local alignment. Choices for amino acid sequences are:

- 'PAM40'
- 'PAM250'
- 'DAYHOFF'
- 'GONNET'
- 'BLOSUM30' increasing by 5 up to 'BLOSUM90'
- 'BLOSUM62'
- 'BLOSUM100'

Default is:

- 'BLOSUM50' (when *AlphabetValue* equals 'AA')
- 'NUC44' (when *AlphabetValue* equals 'NT')

Note All of the above scoring matrices have a built-in scale factor that returns *Score* in bits.

ScaleValue Scale factor used to return *Score* in arbitrary units other than bits. Choices are any positive value. For example, if you enter `log(2)` for *ScaleValue*, then `swalign` returns *Score* in nats.

GapOpenValue Penalty for opening a gap in the alignment. Choices are any positive integer. Default is `8`.

ExtendGapValue	Penalty for extending a gap. Choices are any positive integer. Default is equal to *GapOpenValue*.
ShowscoreValue	Controls the display of the scoring space and the winning path of the alignment. Choices are `true` or `false` (default).

Return Values

Score	Optimal local alignment score in bits.
Alignment	3-by-N character array showing the two sequences, *Seq1* and *Seq2*, in the first and third rows, and symbols representing the optimal local alignment between them in the second row.
Start	2-by-1 vector of indices indicating the starting point in each sequence for the alignment.

Description

`Score = swalign(Seq1, Seq2)` returns the optimal local alignment score in bits. The scale factor used to calculate the score is provided by the scoring matrix.

`[Score, Alignment] = swalign(Seq1, Seq2)` returns a 3-by-N character array showing the two sequences, *Seq1* and *Seq2*, in the first and third rows, and symbols representing the optimal local alignment between them in the second row. The symbol `|` indicates amino acids or nucleotides that match exactly. The symbol `:` indicates amino acids or nucleotides that are related as defined by the scoring matrix (nonmatches with a zero or positive scoring matrix value).

`[Score, Alignment, Start] = swalign(Seq1, Seq2)` returns a 2-by-1 vector of indices indicating the starting point in each sequence for the alignment.

`... = swalign(`*`Seq1`*`,`*`Seq2`*`, ...'`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `swalign` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = swalign(`*`Seq1`*`,`*`Seq2`*`, ...'Alphabet', `*`AlphabetValue`*`)` specifies the type of sequences. Choices are `'AA'` (default) or `'NT'`.

`... = swalign(`*`Seq1`*`,`*`Seq2`*`, ...'ScoringMatrix', `*`ScoringMatrixValue`*`, ...)` specifies the scoring matrix to use for the local alignment. Default is:

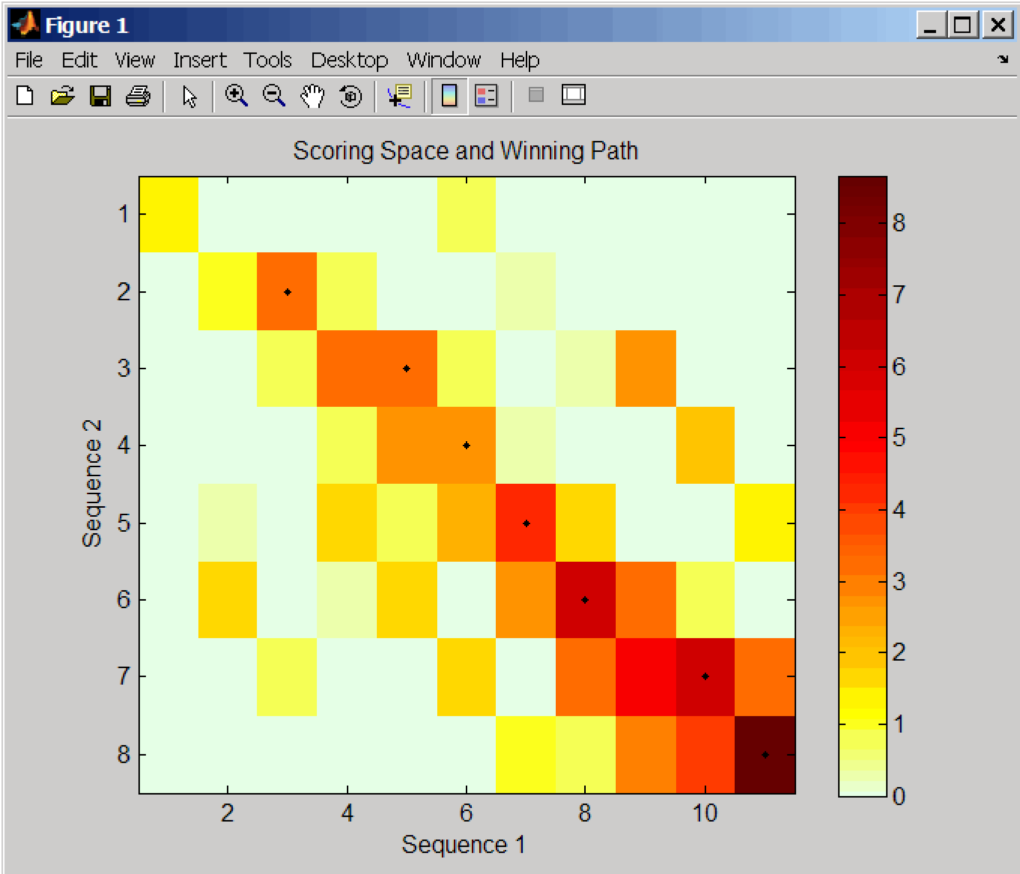
- `'BLOSUM50'` (when *`AlphabetValue`* equals `'AA'`)
- `'NUC44'` (when *`AlphabetValue`* equals `'NT'`)

`... = swalign(`*`Seq1`*`,`*`Seq2`*`, ...'Scale', `*`ScaleValue`*`, ...)` specifies the scale factor used to return *`Score`* in arbitrary units other than bits. Choices are any positive value.

`... = swalign(`*`Seq1`*`,`*`Seq2`*`, ...'GapOpen', `*`GapOpenValue`*`, ...)` specifies the penalty for opening a gap in the alignment. Choices are any positive integer. Default is `8`.

`... = swalign(`*`Seq1`*`,`*`Seq2`*`, ...'ExtendGap', `*`ExtendGapValue`*`, ...)` specifies the penalty for extending a gap in the alignment. Choices are any positive integer. Default is equal to *`GapOpenValue`*.

`... = swalign(`*`Seq1`*`,`*`Seq2`*`, ...'Showscore', `*`ShowscoreValue`*`, ...)` controls the display of the scoring space and winning path of the alignment. Choices are `true` or `false` (default)



The scoring space is a heat map displaying the best scores for all the partial alignments of two sequences. The color of each (`n1,n2`) coordinate in the scoring space represents the best score for the pairing of subsequences `Seq1(s1:n1)` and `Seq2(s2:n2)`, where `n1` is a position in `Seq1`, `n2` is a position in `Seq2`, `s1` is any position in `Seq1` between `1:n1`, and `s2` is any position in `Seq2` between `1:n2`. The best score for a pairing of specific subsequences is determined by scoring all possible alignments of the subsequences by summing matches and gap penalties.

The winning path is represented by black dots in the scoring space and represents the pairing of positions in the optimal local alignment. The color of the last point (lower right) of the winning path represents the optimal local alignment score for the two sequences and is the *Score* output returned by swalign.

Tip The scoring space visually shows tandem repeats, small segments that potentially align, and partial alignments of domains from rearranged sequences.

Examples

1 Locally align two amino acid sequences using the BLOSUM50 (default) scoring matrix and the default values for the GapOpen and ExtendGap properties. Return the optimal local alignment score in bits and the alignment character array. Return the optimal global alignment score in bits and the alignment character array.

```
[Score, Alignment] = swalign('VSPAGMASGYD','IPGKASYD')

Score =

     8.6667

Alignment =

PAGMASGYD
| | || ||
P-GKAS-YD
```

2 Locally align two amino acid sequences specifying the PAM250 scoring matrix and a gap open penalty of 5.

```
[Score, Alignment] = swalign('HEAGAWGHEE','PAWHEAE',...
                             'ScoringMatrix', 'pam250',...
                             'GapOpen',5)
```

```
Score =

     8
Alignment =

GAWGHE
:|| ||
PAW-HE
```

3 Locally align two amino acid sequences returning the *Score* in nat units (nats) by specifying a scale factor of `log(2)`.

```
[Score, Alignment] = swalign('HEAGAWGHEE','PAWHEAE','Scale',log(2))

Score =

    6.4694

Alignment =

AWGHE
|| ||
AW-HE
```

References

[1] Durbin, R., Eddy, S., Krogh, A., and Mitchison, G. (1998). Biological Sequence Analysis (Cambridge University Press).

[2] Smith, T., and Waterman, M. (1981). Identification of common molecular subsequences. Journal of Molecular Biology *147*, 195–197.

See Also

Bioinformatics Toolbox functions: `blosum`, `nt2aa`, `nwalign`, `pam`, `seqdotplot`, `showalignment`

Purpose

Draw nucleotide trace plots

Syntax

```
traceplot(TraceStructure)
traceplot(A, C, G, T)
h = traceplot()
```

Description

`traceplot(TraceStructure)` creates a trace plot from data in a structure with fields `A`, `C`, `G`, `T`.

`traceplot(A, C, G, T)` creates a trace plot from data in vectors `A`, `C`, `G`, `T`.

`h = traceplot()` returns a structure with the handles of the lines corresponding to `A`, `C`, `G`, `T`.

Examples

```
tstruct = scfread('sample.scf');
traceplot(tstruct)
```

See Also

Bioinformatics Toolbox

- function — `scfread`

Methods — By Category

Phylogenetic Tree

Following are methods for use with a `phytree object`.

get (phytree)	Information about phylogenetic tree object
getbyname (phytree)	Branches and leaves from phytree object
getcanonical (phytree)	Calculate canonical form of phylogenetic tree
getmatrix (phytree)	Convert phytree object into relationship matrix
getnewickstr (phytree)	Create Newick-formatted string
pdist (phytree)	Calculate pair-wise patristic distances in phytree object

plot (phytree)	Draw phylogenetic tree
prune (phytree)	Remove branch nodes from phylogenetic tree
reorder (phytree)	Reorder leaves of phylogenetic tree
reroot (phytree)	Change root of phylogenetic tree
select (phytree)	Select tree branches and leaves in phytree object
subtree (phytree)	Extract phylogenetic subtree
view (phytree)	View phylogenetic tree
weights (phytree)	Calculate weights for phylogenetic tree

Graph Visualization

Following are methods for use with a `biograph object`.

allshortestpaths (biograph)	Find all shortest paths in biograph object
conncomp (biograph)	Find strongly or weakly connected components in biograph object
dolayout (biograph)	Calculate node positions and edge trajectories
getancestors (biograph)	Find ancestors in biograph object
getdescendants (biograph)	Find descendants in biograph object
getedgesbynodeid (biograph)	Get handles to edges in biograph object
getmatrix (biograph)	Get connection matrix from biograph object
getnodesbyid (biograph)	Get handles to nodes
getrelatives (biograph)	Find relatives in biograph object

isdag (biograph)	Test for cycles in biograph object
isomorphism (biograph)	Find isomorphism between two biograph objects
isspantree (biograph)	Determine if tree created from biograph object is spanning tree
maxflow (biograph)	Calculate maximum flow and minimum cut in biograph object
minspantree (biograph)	Find minimal spanning tree in biograph object
shortestpath (biograph)	Solve shortest path problem in biograph object
topoorder (biograph)	Perform topological sort of directed acyclic graph extracted from biograph object
traverse (biograph)	Traverse biograph object by following adjacent nodes
view (biograph)	Draw figure from biograph object

Gene Ontology

Following are methods for use with a `geneont object`.

getancestors (geneont)	Numeric IDs for ancestors of Gene Ontology term
getdescendants (geneont)	Numeric IDs for descendants of Gene Ontology term
getmatrix (geneont)	Convert geneont object into relationship matrix
getrelatives (geneont)	Numeric IDs for relatives of Gene Ontology term

Methods — Alphabetical List

allshortestpaths (biograph)

Purpose

Find all shortest paths in biograph object

Syntax

```
[dist] = allshortestpaths(BGObj)
[dist] = allshortestpaths(BGObj, ...'Directed',
DirectedValue, ...)
[dist] = allshortestpaths(BGObj, ...'Weights', WeightsValue,
    ...)
```

Arguments

BGObj	biograph object created by `biograph` (object constructor).
DirectedValue	Property that indicates whether the graph is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.
WeightsValue	Column vector that specifies custom weights for the edges in the N-by-N adjacency matrix extracted from a biograph object, *BGObj*. It must have one entry for every nonzero value (edge) in the matrix. The order of the custom weights in the vector must match the order of the nonzero values in the matrix when it is traversed column-wise. This property lets you use zero-valued weights. By default, `allshortestpaths` gets weight information from the nonzero entries in the matrix.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`[`*`dist`*`] = allshortestpaths(`*`BGObj`*`)` finds the shortest paths between every pair of nodes in a graph represented by an N-by-N adjacency matrix extracted from a biograph object, *BGObj*, using Johnson's algorithm. Nonzero entries in the matrix represent the weights of the edges.

Output `dist` is an N-by-N matrix where `dist(S,T)` is the distance of the shortest path from node `S` to node `T`. A `0` in this matrix indicates the source node; an `Inf` is an unreachable node.

Johnson's algorithm has a time complexity of `O(N*log(N)+N*E)`, where `N` and `E` are the number of nodes and edges respectively.

`[...] = allshortestpaths (BGObj, 'PropertyName', PropertyValue, ...)` calls `allshortestpaths` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[dist] = allshortestpaths(BGObj, ...'Directed', DirectedValue, ...)` indicates whether the graph is directed or undirected. Set `DirectedValue` to `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.

`[dist] = allshortestpaths(BGObj, ...'Weights', WeightsValue, ...)` lets you specify custom weights for the edges. `WeightsValue` is a column vector having one entry for every nonzero value (edge) in the N-by-N adjacency matrix extracted from a biograph object, `BGObj`. The order of the custom weights in the vector must match the order of the nonzero values in the N-by-N adjacency matrix when it is traversed column-wise. This property lets you use zero-valued weights. By default, `allshortestpaths` gets weight information from the nonzero entries in the N-by-N adjacency matrix.

References

[1] Johnson, D.B. (1977). Efficient algorithms for shortest paths in sparse networks. Journal of the ACM *24(1)*, 1-13.

[2] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphallshortestpaths`

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `conncomp`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`, `traverse`

Purpose

Find strongly or weakly connected components in biograph object

Syntax

```
[S, C] = conncomp(BGObj)
[S, C] = conncomp(BGObj, ...'Directed', DirectedValue, ...)
[S, C] = conncomp(BGObj, ...'Weak', WeakValue, ...)
```

Arguments

BGObj	biograph object created by `biograph` (object constructor).
DirectedValue	Property that indicates whether the graph is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`. A DFS-based algorithm computes the connected components. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.
WeakValue	Property that indicates whether to find weakly connected components or strongly connected components. A weakly connected component is a maximal group of nodes that are mutually reachable by violating the edge directions. Set *WeakValue* to `true` to find weakly connected components. Default is `false`, which finds strongly connected components. The state of this parameter has no effect on undirected graphs because weakly and strongly connected components are the same in undirected graphs. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

Description

Tip For introductory information on graph theory functions, see “Graph Theory Functions” in the Bioinformatics Toolbox documentation.

[*S*, *C*] = conncomp(*BGObj*) finds the strongly connected components of an N-by-N adjacency matrix extracted from a biograph object, *BGObj* using Tarjan's algorithm. A strongly connected component is a maximal group of nodes that are mutually reachable without violating the edge directions. The N-by-N sparse matrix represents a directed graph; all nonzero entries in the matrix indicate the presence of an edge.

The number of components found is returned in *S*, and *C* is a vector indicating to which component each node belongs.

Tarjan's algorithm has a time complexity of O(N+E), where N and E are the number of nodes and edges respectively.

[*S*, *C*] = conncomp(*BGObj*, ...'*PropertyName*', *PropertyValue*, ...) calls conncomp with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

[*S*, *C*] = conncomp(*BGObj*, ...'Directed', *DirectedValue*, ...) indicates whether the graph is directed or undirected. Set *directedValue* to false for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is true. A DFS-based algorithm computes the connected components. Time complexity is O(N+E), where N and E are number of nodes and edges respectively.

[*S*, *C*] = conncomp(*BGObj*, ...'Weak', *WeakValue*, ...) indicates whether to find weakly connected components or strongly connected components. A weakly connected component is a maximal group of nodes that are mutually reachable by violating the edge directions. Set *WeakValue* to true to find weakly connected components. Default is false, which finds strongly connected components. The state of this parameter has no effect on undirected graphs because weakly and strongly connected components are the same in undirected graphs. Time complexity is O(N+E), where N and E are number of nodes and edges respectively.

Note By definition, a single node can be a strongly connected component.

Note A directed acyclic graph (DAG) cannot have any strongly connected components larger than one.

References

[1] Tarjan, R.E., (1972). Depth first search and linear graph algorithms. SIAM Journal on Computing *1(2)*, 146–160.

[2] Sedgewick, R., (2002). Algorithms in C++, Part 5 Graph Algorithms (Addison-Wesley).

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphconncomp`

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`, `traverse`

dolayout (biograph)

Purpose

Calculate node positions and edge trajectories

Syntax

```
dolayout(BGobj)
dolayout(BGobj, 'Paths', PathsOnlyValue)
```

Arguments

BGobj	Biograph object created by the `biograph` function (object constructor).
PathsOnlyValue	Controls the calculation of only the edge paths, leaving the nodes at their current positions. Choices are `true` or `false` (default).

Description

`dolayout(`*BGobj*`)` calls the layout engine to calculate the optimal position for each node so that its 2-D rendering is clean and uncluttered, and then calculates the best curves to represent the edges. The layout engine uses the following properties of the biograph object:

- `LayoutType` — Specifies the layout engine as `'hierarchical'`, `'equilibrium'`, or `'radial'`.
- `LayoutScale` — Rescales the sizes of the node before calling the layout engine. This gives more space to the layout and reduces the overlapping of nodes.
- `NodeAutoSize` — Controls precalculating the node size before calling the layout engine. When `NodeAutoSize` is set to `'on'`, the layout engine uses the node properties `FontSize` and `Shape`, and the biograph object property `LayoutScale` to precalculate the actual size of each node. When `NodeAutoSize` is set to `'off'`, the layout engine uses the node property `Size`.

For more information on the above properties, see Properties of a Biograph Object on page 5-4. For information on accessing and specifying the above properties of a biograph object, see and .

`dolayout(BGobj, 'Paths', PathsOnlyValue)` controls the calculation of only the edge paths, leaving the nodes at their current positions. Choices are `true` or `false` (default).

Examples

1 Create a biograph object.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
bg = biograph(cm)
Biograph object with 5 nodes and 9 edges.
bg.nodes(1).Position

ans =

     []
```

Nodes do not have a position yet.

2 Call the layout engine and render the graph.

```
dolayout(bg)
bg.nodes(1).Position

ans =

   112   224

view(bg)
```

3 Manually modify a node position and recalculate the paths only.

```
bg.nodes(1).Position = [150 150];
dolayout(bg, 'Pathsonly', true)
view(bg)
```

See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

MATLAB functions: `get`, `set`

Purpose

Information about phylogenetic tree object

Syntax

```
[Value1, Value2,...] = get(Tree,
'Property1','Property2',...)
get(Tree)
V = get(Tree)
```

Arguments

Tree	Phytree object created with the function `phytree`.
Name	Property name for a `phytree` object.

Description

`[Value1, Value2,...] = get(Tree, 'Property1','Property2',...)` returns the specified properties from a phytree object (`Tree`).

Properties for a `phytree` object are listed in the following table.

Property	Description
`NumLeaves`	Number of leaves
`NumBranches`	Number of branches
`NumNodes`	Number of nodes (`NumLeaves + NumBranches`)
`Pointers`	Branch to leaf/branch connectivity list
`Distances`	Edge length for every leaf/branch
`LeafNames`	Names of the leaves
`BranchNames`	Names of the branches
`NodeNames`	Names of all the nodes

`get(Tree)` displays all property names and their current values for a phytree object (*Tree*).

get (phytree)

`V = get(Tree)` returns a structure where each field name is the name of a property of a phytree object (`Tree`) and each field contains the value of that property.

Examples

1 Read in a phylogenetic tree from a file.

```
tr = phytreeread('pf00002.tree')
```

2 Get the names of the leaves.

```
protein_names = get(tr,'LeafNames')

protein_names =

    'BAI2_HUMAN/917-1197'
    'BAI1_HUMAN/944-1191'
    'O00406/622-883'
     ...
```

See Also

Bioinformatics Toolbox

- functions — `phytree` (object constructor), `phytreeread`
- `phytree` object methods — `getbyname`, `select`

Purpose

Find ancestors in biograph object

Syntax

```
Nodes = getancestors(BiographNode)
Nodes = getancestors(BiographNode, NumGenerations)
```

Arguments

BiographNode	Node in a biograph object.
NumGenerations	Number of generations. Enter a positive integer.

Description

Nodes = getancestors(*BiographNode*) returns a node (BiographNode) and all of its direct ancestors.

Nodes = getancestors(*BiographNode, NumGenerations*) finds the node (*BiographNode*) and its direct ancestors up to a specified number of generations (*NumGenerations*).

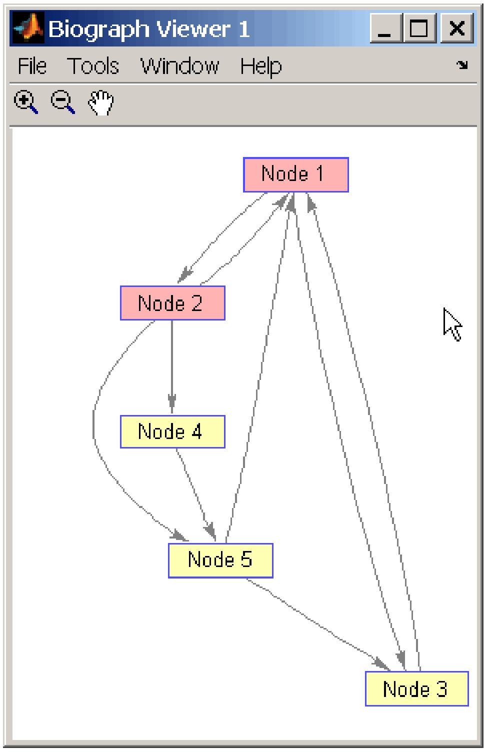
Examples

1 Create a biograph object.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
bg = biograph(cm)
```

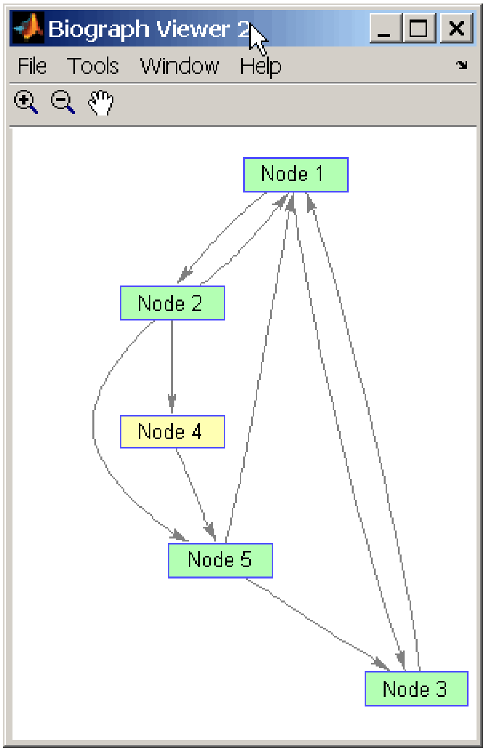
2 Find one generation of ancestors for node 2.

```
ancNodes = getancestors(bg.nodes(2));
set(ancNodes,'Color',[1 .7 .7]);
bg.view;
```



3 Find two generations of ancestors for node 2.

```
ancNodes = getancestors(bg.nodes(2),2);
set(ancNodes,'Color',[.7 1 .7]);
bg.view;
```



See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

MATLAB functions: `get`, `set`

getancestors (geneont)

Purpose

Numeric IDs for ancestors of Gene Ontology term

Syntax

```
AncestorIDs = getancestors(GeneontObj, ID)
AncestorIDs = getancestors(..., 'Height', HeightValue, ...)
```

Description

`AncestorIDs = getancestors(GeneontObj, ID)` returns the numeric IDs (*AncestorIDs*) for the ancestors of a term (*ID*) including the ID for the term. *ID* is a nonnegative integer or a numeric vector with a set of IDs.

`AncestorIDs = getancestors(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`AncestorIDs = getancestors(..., 'Height', HeightValue, ...)` searches up through a specified number of levels (*HeightValue*) in the Gene Ontology database. *HeightValue* is a positive integer. Default is `Inf`.

Examples

1. Download the Gene Ontology database from the Web into MATLAB.

```
GO = geneont('LIVE', true);
```

MATLAB creates a `geneont` object and displays the number of terms in the database.

```
Gene Ontology object with 20005 Terms.
```

2. Get the ancestors for a Gene Ontology term.

```
ancestors = getancestors(GO,46680)

ancestors =
        8150
        9628
        9636
       17085
       42221
```

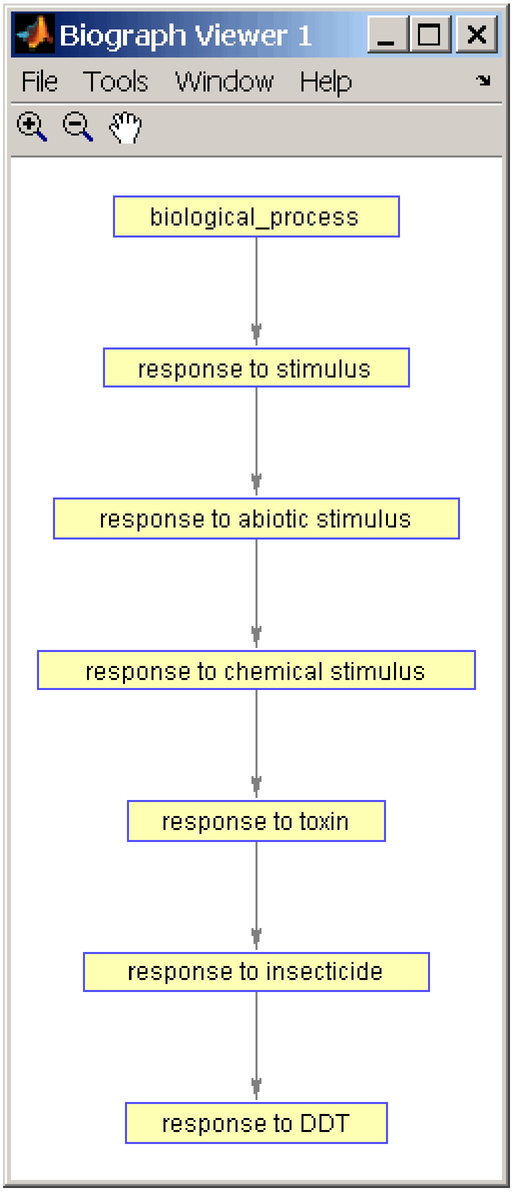
```
46680
50896
```

3 Create a sub Gene Ontology.

```
subontology = GO(ancestors)

Gene Ontology object with 7 Terms.
```

4 View relationships using the biograph functions.

```
[cm acc rels] = getmatrix(subontology);
BG = biograph(cm, get(subontology.Terms, 'name'))
view(BG)
```


Biograph Viewer 1
File
Tools
Window
Help
biological_process
response to stimulus
response to abiotic stimulus
response to chemical stimulus
response to toxin
response to insecticide
response to DDT

See Also

Bioinformatics Toolbox

- functions — `geneont` (object constructor), `goannotread`, `num2goid`
- `geneont` object methods — `getdescendants`, `getmatrix`, `getrelatives`

getbyname (phytree)

Purpose

Branches and leaves from phytree object

Syntax

```
S = getbyname(Tree, Expression)
S = getbyname(Tree, String, 'Exact', true)
```

Arguments

Tree	phytree object created by `phytree` function (object constructor).
Expression	Regular expression. When *Expression* is a cell array of strings, `getbyname` returns a matrix where every column corresponds to every query in *Expression*. For information about the symbols that you can use in a matching regular expression, see the MATLAB function `regexp`.
String	String or cell array of strings.

Description

`S = getbyname(Tree, Expression)` returns a logical vector (*S*) of size `NumNodes`-by-1 with the node names of a phylogenetic tree (*Tree*) that match the regular expression (*Expression*) regardless of letter case.

`S = getbyname(Tree, String, 'Exact', true)` looks for exact string matches and ignores case. When *String* is a cell array of char strings, `getbyname` returns a vector with indices.

Examples

1 Load a phylogenetic tree created from a protein family.

```
tr = phytreeread('pf00002.tree');
```

2 Select all the 'mouse' and 'human' proteins.

```
sel = getbyname(tr,{'mouse','human'});
view(tr,any(sel,2));
```

See Also

Bioinformatics Toolbox

- function — `phytree` (object constructor)
- `phytree` object methods — `get`, `prune`, `select`

getcanonical (phytree)

Purpose

Calculate canonical form of phylogenetic tree

Syntax

```
Pointers = getcanonical(Tree)
[Pointers, Distances, Names] = getcanonical(Tree)
```

Arguments

Tree	phytree object created by `phytree` function (object constructor).

Description

`Pointers` `= getcanonical(`*`Tree`*`)` returns the pointers for the canonical form of a phylogenetic tree (*`Tree`*). In a canonical tree the leaves are ordered alphabetically and the branches are ordered first by their width and then alphabetically by their first element. A canonical tree is isomorphic to all the trees with the same skeleton independently of the order of their leaves and branches.

`[`*`Pointers, Distances, Names`*`] = getcanonical(`*`Tree`*`)` returns, in addition to the pointers described above, the reordered distances (*`Distances`*) and node names (*`Names`*).

Examples

1. Create two phylogenetic trees with the same skeleton but slightly different distances.

```
b = [1 2; 3 4; 5 6; 7 8;9 10];
tr_1 = phytree(b,[.1 .2 .3 .3 .4 ]');
tr_2 = phytree(b,[.2 .1 .2 .3 .4 ]');
```

2. Plot the trees.

```
plot(tr_1)
plot(tr_2)
```

3. Check whether the trees have an isomorphic construction.

```
isequal(getcanonical(tr_1),getcanonical(tr_2))
```

```
ans =
     1
```

See Also

Bioinformatics Toolbox

- functions — `phytree` (object constructor), `phytreeread`
- `phytree` object methods — `getbyname`, `select`, `subtree`

getdescendants (biograph)

Purpose

Find descendants in biograph object

Syntax

Nodes = getdescendants(*BiographNode*)
Nodes = getdescendants(*BiographNode*,*NumGenerations*)

Arguments

BiographNode	Node in a biograph object.
NumGenerations	Number of generations. Enter a positive integer.

Description

Nodes = getdescendants(*BiographNode*) finds a given node (*BiographNode*) all of its direct descendants.

Nodes = getdescendants(*BiographNode*,*NumGenerations*) finds the node (*BiographNode*) and all of its direct descendants up to a specified number of generations (*NumGenerations*).

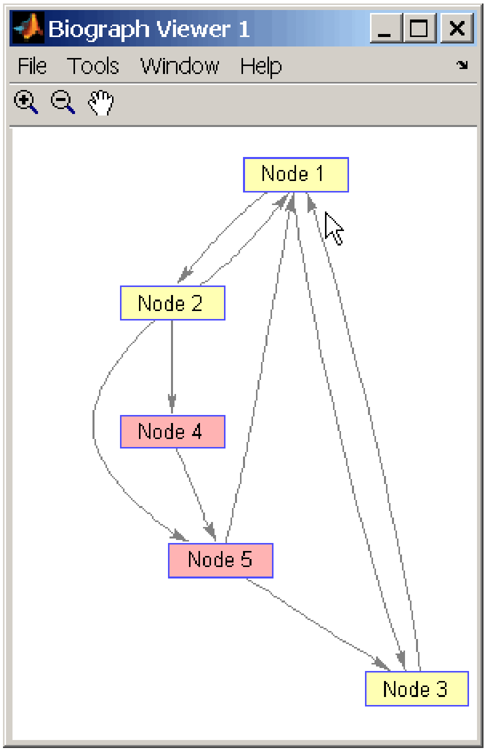
Examples

1 Create a biograph object.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
bg = biograph(cm)
```

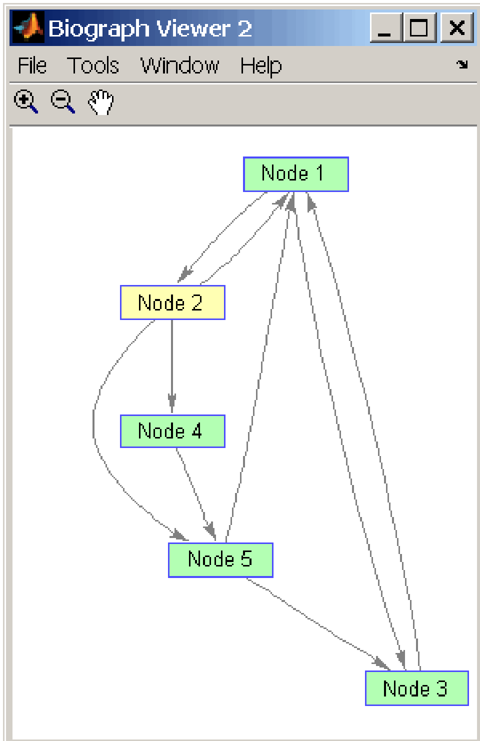
2 Find one generation of descendants for node 4.

```
desNodes = getdescendants(bg.nodes(4));
set(desNodes,'Color',[1 .7 .7]);
bg.view;
```



3 Find two generations of descendants for node 4.

```
desNodes = getdescendants(bg.nodes(4),2);
set(desNodes,'Color',[.7 1 .7]);
bg.view;
```



See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

MATLAB functions: `get`, `set`

Purpose

Numeric IDs for descendants of Gene Ontology term

Syntax

DescendantIDs = getdescendants(*GeneontObj*, *ID*)
DescendantIDs = getdescendants(..., 'Depth', *DepthValue*,...)

Description

DescendantIDs = getdescendants(*GeneontObj*, *ID*) returns the numeric IDs (*DescendantIDs*) for the descendants of a term (*ID*) including the ID for the term. *ID* is a nonnegative integer or a numeric vector with a set of IDs.

DescendantIDs = getdescendants(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

DescendantIDs = getdescendants(..., 'Depth', *DepthValue*,...) searches down through a specified number of levels (*DepthValue*) in the Gene Ontology. *DepthValue* is a positive integer. Default is Inf.

Examples

1. Download the Gene Ontology database from the Web into MATLAB.

   ```
   GO = geneont('LIVE', true);
   ```

   MATLAB creates a geneont object and displays the number of terms in the database.

   ```
   Gene Ontology object with 20005 Terms.
   ```

2. Get the ancestors for a Gene Ontology term.

   ```
   descendants = getdescendants(GO,5622, 'Depth', 5)
   ```

3. Create a sub Gene Ontology.

   ```
   subontology = GO(descendants)

   Gene Ontology object with 1071 Terms.
   ```

See Also

Bioinformatics Toolbox

- functions — `geneont` (object constructor), `goannotread`, `num2goid`
- `geneont` object methods — `getancestors`, `getmatrix`, `getrelatives`

Purpose Get handles to edges in biograph object

Syntax *Edges* = getedgesbynodeid(*BGobj*,*SourceIDs*,*SinkIDs*)

Arguments

BGobj	Biograph object.
SourceIDs, *SinkIDs*	Enter a cell string, or an empty cell array (gets all edges).

Description *Edges* = getedgesbynodeid(*BGobj*,*SourceIDs*,*SinkIDs*) gets the handles to the edges that connect the specified source nodes (*SourceIDs*) to the specified sink nodes (*SinkIDs*) in a biograph object.

Example

1 Create a biograph object for the Hominidae family.

```
species = {'Homo','Pan','Gorilla','Pongo','Baboon',...
           'Macaca','Gibbon'};
cm = magic(7)>25 & 1-eye(7);
bg = biograph(cm, species);
```

2 Find all the edges that connect to the Homo node.

```
EdgesIn = getedgesbynodeid(bg,[],'Homo');
EdgesOut = getedgesbynodeid(bg,'Homo',[]);
set(EdgesIn,'LineColor',[0 1 0]);
set(EdgesOut,'LineColor',[1 0 0]);
bg.view;
```

3 Find all edges that connect members of the Cercopithecidae family to members of the Hominidae family.

```
Cercopithecidae = {'Macaca','Baboon'};
Hominidae = {'Homo','Pan','Gorilla','Pongo'};
edgesSel = getedgesbynodeid(bg,Cercopithecidae,Hominidae);
set(bg.edges,'LineColor',[.5 .5 .5]);
set(edgesSel,'LineColor',[0 0 1]);
```

```
bg.view;
```

See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

MATLAB functions: `get`, `set`

Purpose

Get connection matrix from biograph object

Syntax

`[Matrix, ID, Distances] = getmatrix(BGObj)`

Arguments

BGObj	biograph object created by `biograph` (object constructor).

Description

`[Matrix, ID, Distances] = getmatrix(BGObj)` converts the biograph object, *BiographObj*, into a logical sparse matrix, *Matrix*, in which 1 indicates that a node (row index) is connected to another node (column index). *ID* is a cell array of strings listing the `ID` properties for each node, and corresponds to the rows and columns of *Matrix*. *Distances* is a column vector with one entry for every nonzero entry in *Matrix* traversed column-wise and representing the respective `Weight` property for each edge.

Examples

```
cm = [0 1 1 0 0;2 0 0 4 4;4 0 0 0 0;0 0 0 0 2;4 0 5 0 0];
bg = biograph(cm);
[cm, IDs, dist] = getmatrix(bg)
```

See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

getmatrix (geneont)

Purpose

Convert geneont object into relationship matrix

Syntax

`[Matrix, ID, Relationship] = getmatrix(GeneontObj)`

Arguments

GeneontObj	geneont object created by `geneont` (object constructor)

Description

`[Matrix, ID, Relationship] = getmatrix(GeneontObj)` converts a geneont object, *GeneontObj*, into *Matrix*, a matrix of relationship values between nodes (row and column indices), in which 0 indicates no relationship, 1 indicates an "is_a" relationship, and 2 indicates a "part_of" relationship. *ID* is a column vector listing Gene Ontology IDs that correspond to the rows and columns of *Matrix*. *Relationship* is a cell array of strings defining the types of relationships.

Examples

```
GO = geneont('LIVE',true);
[MATRIX, ID, REL] = getmatrix(GO);
```

See Also

- Bioinformatics Toolbox functions — `geneont` (object constructor), `goannotread`, `num2goid`
- Bioinformatics Toolbox object — `geneont object`
- Bioinformatics Toolbox methods of `geneont object` — `getancestors`, `getdescendants`, `getmatrix`, `getrelatives`

Purpose

Convert phytree object into relationship matrix

Syntax

`[Matrix, ID, Distances] = getmatrix(PhytreeObj)`

Arguments

PhytreeObj	phytree object created by `phytree` (object constructor).

Description

`[Matrix, ID, Distances] = getmatrix(PhytreeObj)` converts a phytree object, *PhytreeObj*, into a logical sparse matrix, *Matrix*, in which 1 indicates that a branch node (row index) is connected to its child (column index). The child can be either another branch node or a leaf node. *ID* is a column vector of strings listing the labels that correspond to the rows and columns of *Matrix*, with the labels from 1 to *Number of Leaves* being the leaf nodes, then the labels from *Number of Leaves* + 1 to *Number of Leaves* + *Number of Branches* being the branch nodes, and the label for the last branch node also being the root node. *Distances* is a column vector with one entry for every nonzero entry in *Matrix* traversed column-wise and representing the distance between the branch node and the child.

Examples

```
T = phytreeread('pf00002.tree')
[MATRIX, ID, DIST] = getmatrix(T);
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreetool`

Bioinformatics Toolbox object: `phytree object`

Bioinformatics Toolbox methods of phytree object: `get`, `pdist`, `prune`

getnewickstr (phytree)

Purpose

Create Newick-formatted string

Syntax

```
String = getnewickstr(Tree)
getnewickstr(..., 'PropertyName', PropertyValue,...)
getnewickstr(..., 'Distances', DistancesValue)
getnewickstr(..., 'BranchNames', BranchNamesValue)
```

Arguments

Tree	Phytree object created with the function `phytree`.
DistancesValue	Property to control including or excluding distances in the output. Enter either `true` (include distances) or `false` (exclude distances). Default is `true`.
BranchNamesValue	Property to control including or excluding branch names in the output. Enter either `true` (include branch names) or `false` (exclude branch names). Default is `false`.

Description

String = `getnewickstr(`*Tree*`)` returns the Newick formatted string of a phylogenetic tree object (*Tree*).

`getnewickstr(..., '`*PropertyName*`',` *PropertyValue*`,...)` defines optional properties using property name/value pairs.

`getnewickstr(..., 'Distances',` *DistancesValue*`)`, when *DistancesValue* is `false`, excludes the distances from the output.

`getnewickstr(..., 'BranchNames',` *BranchNamesValue*`)`, when *BranchNamesValue* is `true`, includes the branch names in the output.

References

Information about the Newick tree format.

`http://evolution.genetics.washington.edu/phylip/newicktree.html`

Examples

1 Create some random sequences.

```
seqs = int2nt(ceil(rand(10)*4));
```

2 Calculate pairwise distances.

```
dist = seqpdist(seqs,'alpha','nt');
```

3 Construct a phylogenetic tree.

```
tree = seqlinkage(dist);
```

4 Get the Newick string.

```
str  = getnewickstr(tree)
```

See Also

Bioinformatics Toolbox

- functions — `phytree` (object constructor), `phytreeread`, `phytreetool`, `phytreewrite`, `seqlinkage`
- `phytree` object methods — `get`, `getbyname`, `getcanonical`

getnodesbyid (biograph)

Purpose Get handles to nodes

Syntax *NodesHandles* = getnodesbyid(*BGobj*,*NodeIDs*)

Arguments

BGobj	Biograph object.
NodeIDs	Enter a cell string of node identifications.

Description *NodesHandles* = getnodesbyid(*BGobj*,*NodeIDs*) gets the handles for the specified nodes (*NodeIDs*) in a biograph object.

Example

1 Create a biograph object.

```
species = {'Homosapiens','Pan','Gorilla','Pongo','Baboon',...
           'Macaca','Gibbon'};
cm = magic(7)>25 & 1-eye(7);
bg = biograph(cm, species)
```

2 Find the handles to members of the Cercopithecidae family and members of the Hominidae family.

```
Cercopithecidae = {'Macaca','Baboon'};
Hominidae = {'Homosapiens','Pan','Gorilla','Pongo'};
CercopithecidaeNodes = getnodesbyid(bg,Cercopithecidae);
HominidaeNodes = getnodesbyid(bg,Hominidae);
```

3 Color the families differently and draw a graph.

See Also Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

MATLAB functions: `get`, `set`

getrelatives (biograph)

Purpose

Find relatives in biograph object

Syntax

```
Nodes = getrelatives(BiographNode)
Nodes = getrelatives(BiographNode,NumGenerations)
```

Arguments

BiographNode	Node in a biograph object.
NumGenerations	Number of generations. Enter a positive integer.

Description

Nodes = getrelatives(*BiographNode*) finds all the direct relatives for a given node (*BiographNode*).

Nodes = getrelatives(*BiographNode*,*NumGenerations*) finds the direct relatives for a given node (*BiographNode*) up to a specified number of generations (*NumGenerations*).

Examples

1 Create a biograph object.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
bg = biograph(cm)
```

2 Find all nodes interacting with node 1.

```
intNodes = getrelatives(bg.nodes(1));
set(intNodes,'Color',[.7 .7 1]);
bg.view;
```

See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

MATLAB functions: `get`, `set`

Purpose

Numeric IDs for relatives of Gene Ontology term

Syntax

```
RelativeIDs = getrelatives(GeneontObj, ID)
getrelatives(..., 'PropertyName', PropertyValue,...)
getrelatives(..., 'Height', HeightValue)
getrelatives(..., 'Depth', DepthValue)
```

Arguments

GeneontObj

ID

Description

`RelativeIDs = getrelatives(GeneontObj, ID)` returns the numeric IDs (`RelativeIDs`) for the relatives of a term (`ID`) including the ID for the term. `ID` is a nonnegative integer or a numeric vector with a set of IDs.

`getrelatives(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`getrelatives(..., 'Height', HeightValue)` includes terms that are related up through a specified number of levels (`HeightValue`) in the Gene Ontology database. `HeightValue` is a positive integer. Default is `1`.

`getrelatives(..., 'Depth', DepthValue)` includes terms that are related down through a specified number of levels (`DepthValue`) in the Gene Ontology database. `DepthValue` is a positive integer. Default is `1`.

Examples

1 Download the Gene Ontology database from the Web into MATLAB.

```
GO = geneont('LIVE', true);
```

MATLAB creates a geneont object and displays the number of terms in the database.

```
Gene Ontology object with 20005 Terms.
```

2 Get the relatives for a Gene Ontology term.

```
subontology = getrelatives(GO,46680)
```

See Also

Bioinformatics Toolbox

- functions — `geneont` (object constructor), `goannotread`, `num2goid`
- `geneont` object methods — `getancestors`, `getdescendants`, `getmatrix`

Purpose

Test for cycles in biograph object

Syntax

`isdag(BGObj)`

Arguments

BGObj	biograph object created by `biograph` (object constructor).

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`isdag(BGObj)` returns logical 1 (`true`) if an N-by-N adjacency matrix extracted from a biograph object, *BGObj*, is a directed acyclic graph (DAG) and logical 0 (`false`) otherwise. In the N-by-N sparse matrix, all nonzero entries indicate the presence of an edge.

References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphisdag`

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`, `traverse`

isomorphism (biograph)

Purpose

Find isomorphism between two biograph objects

Syntax

```
[Isomorphic, Map] = isomorphism(BGObj1, BGObj2)
[Isomorphic, Map] = isomorphism(BGObj1, BGObj2,'Directed',
    DirectedValue)
```

Arguments

BGObj1	biograph object created by `biograph` (object constructor).
BGObj2	biograph object created by `biograph` (object constructor).
DirectedValue	Property that indicates whether the graphs are directed or undirected. Enter `false` when both *BGObj1* and *BGObj2* produce undirected graphs. In this case, the upper triangles of the sparse matrices extracted from *BGObj1* and *BGObj2* are ignored. Default is `true`, meaning that both graphs are directed.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`[`*`Isomorphic`*`, `*`Map`*`] = isomorphism(`*`BGObj1`*`, `*`BGObj2`*`)` returns logical 1 (`true`) in *Isomorphic* if two N-by-N adjacency matrices extracted from biograph objects *BGObj1* and *BGObj2* are isomorphic graphs, and logical 0 (`false`) otherwise. A graph isomorphism is a 1-to-1 mapping of the nodes in the graph from *BGObj1* and the nodes in the graph from *BGObj2* such that adjacencies are preserved. Return value *Isomorphic* is Boolean. When *Isomorphic* is `true`, *Map* is a row vector containing the node indices that map from *BGObj2* to *BGObj1*. When *Isomorphic* is `false`, the worst-case time complexity is `O(N!)`, where `N` is the number of nodes.

`[Isomorphic, Map] = isomorphism(BGObj1, BGObj2,'Directed', DirectedValue)` indicates whether the graphs are directed or undirected. Set *DirectedValue* to `false` when both *BGObj1* and *BGObj2* produce undirected graphs. In this case, the upper triangles of the sparse matrices extracted from *BGObj1* and *BGObj2* are ignored. The default is `true`, meaning that both graphs are directed.

References

[1] Fortin, S. (1996). The Graph Isomorphism Problem. Technical Report, 96-20, Dept. of Computer Science, University of Alberta, Edomonton, Alberta, Canada.

[2] McKay, B.D. (1981). Practical Graph Isomorphism. Congressus Numerantium *30*, 45-87.

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphisomorphism`

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isdag`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`, `traverse`

isspantree (biograph)

Purpose

Determine if tree created from biograph object is spanning tree

Syntax

`TF = isspantree(BGObj)`

Arguments

BGObj	biograph object created by `biograph` (object constructor).

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`TF = isspantree(BGObj)` returns logical 1 (`true`) if the N-by-N adjacency matrix extracted from a biograph object, *BGObj*, is a spanning tree, and logical 0 (`false`) otherwise. A spanning tree must touch all the nodes and must be acyclic. The lower triangle of the N-by-N adjacency matrix represents an undirected graph, and all nonzero entries indicate the presence of an edge.

References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphisspantree`

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isdag`, `isomorphism`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`, `traverse`

Purpose

Calculate maximum flow and minimum cut in biograph object

Syntax

```
[MaxFlow, FlowMatrix, Cut] = maxflow(BGObj, SNode, TNode)
[...] = maxflow(BGObj, SNode, TNode, ...'Capacity',
CapacityValue, ...)
[...] = maxflow(BGObj, SNode, TNode, ...'Method', MethodValue,
    ...)
```

Arguments

BGObj	biograph object created by `biograph` (object constructor).
SNode	Node in a directed graph represented by an N-by-N adjacency matrix extracted from biograph object, *BGObj*.
TNode	Node in a directed graph represented by an N-by-N adjacency matrix extracted from biograph object, *BGObj*.

CapacityValue	Column vector that specifies custom capacities for the edges in the N-by-N adjacency matrix. It must have one entry for every nonzero value (edge) in the N-by-N adjacency matrix. The order of the custom capacities in the vector must match the order of the nonzero values in the N-by-N adjacency matrix when it is traversed column-wise. By default, `maxflow` gets capacity information from the nonzero entries in the N-by-N adjacency matrix.
MethodValue	String that specifies the algorithm used to find the minimal spanning tree (MST). Choices are: • `'Edmonds'` — Uses the Edmonds and Karp algorithm, the implementation of which is based on a variation called the *labeling algorithm*. Time complexity is `O(N*E^2)`, where `N` and `E` are the number of nodes and edges respectively. • `'Goldberg'` — Default algorithm. Uses the Goldberg algorithm, which uses the generic method known as *preflow-push*. Time complexity is `O(N^2*sqrt(E))`, where `N` and `E` are the number of nodes and edges respectively.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`[`*`MaxFlow`*`, `*`FlowMatrix`*`, `*`Cut`*`] = maxflow(`*`BGObj`*`, `*`SNode`*`, `*`TNode`*`)` calculates the maximum flow of a directed graph represented by an N-by-N adjacency matrix extracted from a biograph object, *`BGObj`*, from node *SNode* to node *TNode*. Nonzero entries in the matrix determine the capacity of the edges. Output *MaxFlow* is the maximum flow, and *FlowMatrix* is a sparse matrix with all the flow values for every edge. *FlowMatrix*(*X*,*Y*) is the flow from node *X* to node *Y*. Output *Cut* is a logical row vector indicating the nodes connected to *SNode* after calculating the minimum cut between *SNode* and *TNode*. If several solutions to the minimum cut problem exist, then *Cut* is a matrix.

`[...] = maxflow(`*BGObj*`,` *SNode*`,` *TNode*`, ...'`*PropertyName*`',` *PropertyValue*`, ...)` calls `maxflow` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[...] = maxflow(`*BGObj*`,` *SNode*`,` *TNode*`, ...'Capacity',` *CapacityValue*`, ...)` lets you specify custom capacities for the edges. *CapacityValue* is a column vector having one entry for every nonzero value (edge) in the N-by-N adjacency matrix. The order of the custom capacities in the vector must match the order of the nonzero values in the matrix when it is traversed column-wise. By default, `graphmaxflow` gets capacity information from the nonzero entries in the matrix.

`[...] = maxflow(`*BGObj*`,` *SNode*`,` *TNode*`, ...'Method',` *MethodValue*`, ...)` lets you specify the algorithm used to find the minimal spanning tree (MST). Choices are:

- `'Edmonds'` — Uses the Edmonds and Karp algorithm, the implementation of which is based on a variation called the *labeling algorithm*. Time complexity is `O(N*E^2)`, where `N` and `E` are the number of nodes and edges respectively.
- `'Goldberg'` — Default algorithm. Uses the Goldberg algorithm, which uses the generic method known as *preflow-push*. Time complexity is `O(N^2*sqrt(E))`, where `N` and `E` are the number of nodes and edges respectively.

References

[1] Edmonds, J. and Karp, R.M. (1972). Theoretical improvements in the algorithmic efficiency for network flow problems. Journal of the ACM *19*, 248-264.

[2] Goldberg, A.V. (1985). A New Max-Flow Algorithm. MIT Technical Report MIT/LCS/TM-291, Laboratory for Computer Science, MIT.

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphmaxflow`

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isdag`, `isomorphism`, `isspantree`, `minspantree`, `shortestpath`, `topoorder`, `traverse`

Purpose

Find minimal spanning tree in biograph object

Syntax

```
[Tree, pred] = minspantree(BGObj)
[Tree, pred] = minspantree(BGObj, R)
[Tree, pred] = minspantree(..., 'Method', MethodValue, ...)
[Tree, pred] = minspantree(..., 'Weights', WeightsValue, ...)
```

Arguments

BGObj	biograph object created by `biograph` (object constructor).
R	Scalar between 1 and the number of nodes.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`[Tree, pred] = minspantree(BGObj)` finds an acyclic subset of edges that connects all the nodes in the undirected graph represented by an N-by-N adjacency matrix extracted from a biograph object, *BGObj*, and for which the total weight is minimized. Weights of the edges are all nonzero entries in the lower triangle of the N-by-N sparse matrix. Output *Tree* is a spanning tree represented by a sparse matrix. Output *pred* is a vector containing the predecessor nodes of the minimal spanning tree (MST), with the root node indicated by `0`. The root node defaults to the first node in the largest connected component. This computation requires an extra call to the `graphconncomp` function.

`[Tree, pred] = minspantree(BGObj, R)` sets the root of the minimal spanning tree to node `R`.

`[Tree, pred] = minspantree(..., 'PropertyName', PropertyValue, ...)` calls `minspantree` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[Tree, pred] = minspantree(..., 'Method', MethodValue, ...)` lets you specify the algorithm used to find the minimal spanning tree (MST). Choices are:

- `'Kruskal'` — Grows the minimal spanning tree (MST) one edge at a time by finding an edge that connects two trees in a spreading forest of growing MSTs. Time complexity is `O(E+X*log(N))`, where `X` is the number of edges no longer than the longest edge in the MST, and `N` and `E` are the number of nodes and edges respectively.
- `'Prim'` — Default algorithm. Grows the minimal spanning tree (MST) one edge at a time by adding a minimal edge that connects a node in the growing MST with any other node. Time complexity is `O(E*log(N))`, where `N` and `E` are the number of nodes and edges respectively.

Note When the graph is unconnected, Prim's algorithm returns only the tree that contains R, while Kruskal's algorithm returns an MST for every component.

`[Tree, pred] = minspantree(..., 'Weights', WeightsValue, ...)` lets you specify custom weights for the edges. *`WeightsValue`* is a column vector having one entry for every nonzero value (edge) in the N-by-N sparse matrix. The order of the custom weights in the vector must match the order of the nonzero values in the N-by-N sparse matrix when it is traversed column-wise. By default, `minspantree` gets weight information from the nonzero entries in the N-by-N sparse matrix.

References

[1] Kruskal, J.B. (1956). On the Shortest Spanning Subtree of a Graph and the Traveling Salesman Problem. Proceedings of the American Mathematical Society *7*, 48-50.

[2] Prim, R. (1957). Shortest Connection Networks and Some Generalizations. Bell System Technical Journal *36*, 1389-1401.

[3] Siek, J.G. Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphminspantree`

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `shortestpath`, `topoorder`, `traverse`

pdist (phytree)

Purpose Calculate pair-wise patristic distances in phytree object

Syntax

```
D = pdist(Tree)
[D,C] = pdist(Tree)
pdist(..., 'PropertyName', PropertyValue,...)
pdist(..., 'Nodes', NodeValue)
pdist(... , Squareform', SquareformValue)
pdist(..., 'Criteria', CriteriaValue)
```

Arguments

`Tree`	Phylogenetic tree object created with the `phytree` constructor function.
`NodeValue`	Property to select the nodes. Enter either `'leaves'` (default) or `'all'`.
`SquareformValue`	Property to control creating a square matrix.

Description

`D = pdist(Tree)` returns a vector (*D*) containing the patristic distances between every possible pair of leaf nodes a phylogenetic tree object (*Tree*). The patristic distances are computed by following paths through the branches of the tree and adding the patristic branch distances originally created with seqlinkage.

The output vector *D* is arranged in the order `((2,1),(3,1),..., (M,1),(3,2),...(M,3),.....(M,M-1))` (the lower-left triangle of the full `M`-by-`M` distance matrix). To get the distance between the `I`th and `J`th nodes (`I > J`), use the formula `D((J-1)*(M-J/2)+I-J)`. `M` is the number of leaves.

`[D,C] = pdist(Tree)` returns in C the index of the closest common parent nodes for every possible pair of query nodes.

`pdist(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`pdist(..., 'Nodes', NodeValue)` indicates the nodes included in the computation. When `Node='leaves'`, the output is ordered as before, but *M* is the total number of nodes in the tree (`NumLeaves+NumBranches`).

`pdist(...  , Squareform', SquareformValue)`, when Squareform is `true`, converts the output into a square formatted matrix, so that `D(I,J)` denotes the distance between the `I`th and the `J`th nodes. The output matrix is symmetric and has a zero diagonal.

`pdist(..., 'Criteria', CriteriaValue)` changes the criteria used to relate pairs. C can be `'distance'` (default) or `'levels'`.

Examples

1 Get a phylogenetic tree from a file.

```
tr = phytreeread('pf00002.tree')
```

2 Calculate the tree distances between pairs of leaves.

```
dist = pdist(tr,'nodes','leaves','squareform',true)
```

See Also

Bioinformatics Toolbox

- functions — `phytree` (object constructor), `phytreeread`, `phytreetool`, `seqlinkage`, `seqpdist`

plot (phytree)

Purpose

Draw phylogenetic tree

Syntax

```
plot(Tree)
plot(Tree, ActiveBranches)
plot(..., 'Type', TypeValue)
plot(...,'Orientation', OrientationValue)
plot(...,'BranchLabels', BranchLabelsValue)
plot(...,'LeafLabels', LeafLabelsValue)
plot(...,'TerminalLabels', TerminalLabelsValue)
```

Arguments

`Tree`	Phylogenetic tree object created with the `phytree` constructor function.
`ActiveBranches`	Branches veiwable in the figure window.
`TypeValue`	Property to select a method for drawing a phylogenetic tree. Enter `'square'` , `'angular'`, or `'radial'`. The default value is `'square'`.
`OrientationValue`	Property to orient a phylogram or cladogram tree. Enter `'top'`, `'bottom'`, `'left'`, or `'right'`. The default value is `'left'`.
`BranchLabelsValue`	Property to control displaying branch labels. Enter either `true` or `false`. The default value is `false`.
`LeafLabelsValue`	Property to control displaying leaf labels. Enter either `true` or `false`. The default value is `false`.
`TerminalLabels`	Property to control displaying terminal labels. Enter either `true` or `false`. The default value is `false`.

Description

`plot(Tree)` draws a phylogenetic tree object into a MATLAB figure as a phylogram. The significant distances between branches and nodes are in the horizontal direction. Vertical distances have no significance and are selected only for display purposes. Handles to graph elements are stored in the figure field `UserData` so that you can easily modify graphic properties.

`plot(Tree, ActiveBranches)` hides the nonactive branches and all of their descendants. `ActiveBranches` is a logical array of size `numBranches x 1` indicating the active branches.

`plot(..., 'Type', TypeValue)` selects a method for drawing a phylogenetic tree.

`plot(...,'Orientation', OrientationValue)` orients a phylogenetic tree within a figure window. The `Orientation` property is valid only for phylogram and cladogram trees.

`plot(...,'BranchLabels', BranchLabelsValue)` hides or displays branch labels placed next to the branch node.

`plot(...,'LeafLabels', LeafLabelsValue)` hides or displays leaf labels placed next to the leaf nodes.

`plot(...,'TerminalLabels', TerminalLabelsValue)` hides or displays terminal labels. Terminal labels are placed over the axis tick labels and ignored when `Type= 'radial'`.

`H = plot(...)` returns a structure with handles to the graph elements.

Examples

```
tr = phytreeread('pf00002.tree')
plot(tr,'Type','radial')
```

Graph element properties can be modified as follows:

```
h=get(gcf,'UserData')
set(h.branchNodeLabels,'FontSize',6,'Color',[.5 .5 .5])
```

See Also

Bioinformatics Toolbox

- functions — `phytree` (object constructor), `phytreeread`, `phytreetool`, `seqlinkage`

- phytree object method — view

Purpose

Remove branch nodes from phylogenetic tree

Syntax

```
T2 = prune(T1, Nodes)
T2 = prune(T1, Nodes, 'Mode','Exclusive')
```

Arguments

T1	Phylogenetic object created with the phytree constructor function.
Nodes	Nodes to remove from tree.
Mode	Property to control the method of pruning. Enter either 'Inclusive' or 'Exclusive'. The default value is 'Inclusive'.

Description

T2 = prune(T1, Nodes)removes the nodes listed in the vector Nodes from the tree T1. prune removes any branch or leaf node listed in Nodes and all their descendants from the tree T1, and returns the modified tree T2. The parent nodes are connected to the 'brothers' as required. Nodes in the tree are labeled as [1:numLeaves] for the leaves and as [numLeaves+1:numLeaves+numBranches] for the branches. Nodes can also be a logical array of size [numLeaves+numBranches x 1] indicating the nodes to be removed.

T2 = prune(T1, Nodes, 'Mode','Exclusive')changes the property (Mode) for pruning to 'Exclusive' and removes only the descendants of the nodes listed in the vector Nodes. Nodes that do not have a predecessor become leaves in the list Nodes. In this case, pruning is the process of reducing a tree by turning some branch nodes into leaf nodes, and removing the leaf nodes under the original branch.

Examples

Load a phylogenetic tree created from a protein family

```
tr = phytreeread('pf00002.tree');
view(tr)
                % To :
```

Remove all the 'mouse' proteins

```
ind = getbyname(tr,'mouse');
tr = prune(tr,ind);
view(tr)
```

Remove potential outliers in the tree

```
[sel,sel_leaves] = select(tr,'criteria','distance',...
                             'threshold',.3,...
                             'reference','leaves',...
                             'exclude','leaves',...
                             'propagate','toleaves');
tr = prune(tr,~sel_leaves)
view(tr)
```

See Also

Bioinformatics Toolbox

- functions — `phytree` (object constructor), `phytreetool`
- `phytree` object methods — `select`, `get`

Purpose

Reorder leaves of phylogenetic tree

Syntax

```
Tree1Reordered = reorder(Tree1, Order)
[Tree1Reordered, OptimalOrder] = reorder(Tree1, Order,
   'Approximate', ApproximateValue)
[Tree1Reordered, OptimalOrder] = reorder(Tree1, Tree2)
```

Arguments

Tree1, *Tree2*	Phytree objects.
Order	Vector with position indices for each leaf.
ApproximateValue	Controls the use of the optimal leaf-ordering calculation to find the closest order possible to the suggested one without dividing the clades or producing crossing branches. Enter `true` to use the calculation. Default is `false`.

Return Values

Tree1Reordered	Phytree object with reordered leaves.
OptimalOrder	Vector of position indices for each leaf in *Tree1Reordered*, determined by the optimal leaf-ordering calculation.

Description

Tree1Reordered = `reorder(`*Tree1*, *Order*`)` reorders the leaves of the phylogenetic tree *Tree1*, without modifying its structure and distances, creating a new phylogenetic tree, *Tree1Reordered*. *Order* is a vector of position indices for each leaf. If *Order* is invalid, that is, if it divides the clades (or produces crossing branches), then `reorder` returns an error message.

[*Tree1Reordered*, *OptimalOrder*] = `reorder(`*Tree1*, *Order*, `'Approximate'`, *ApproximateValue*`)` controls the use of the optimal leaf-ordering calculation, which finds the best approximate order closest to the suggested one, without dividing the clades or producing crossing branches. Enter `true` to use the calculation and return

`Tree1Reordered`, the reordered tree, and *`OptimalOrder`*, a vector of position indices for each leaf in *`Tree1Reordered`*, determined by the optimal leaf-ordering calculation. Default is `false`.

`[`*`Tree1Reordered`*`, `*`OptimalOrder`*`] = reorder(`*`Tree1`*`, `*`Tree2`*`)` uses the optimal leaf-ordering calculation to reorder the leaves in *`Tree1`* such that it matches the order of leaves in *`Tree2`* as closely as possible, without dividing the clades or producing crossing branches. *`Tree1Reordered`* is the reordered tree, and *`OptimalOrder`* is a vector of position indices for each leaf in *`Tree1Reordered`*, determined by the optimal leaf-ordering calculation

Examples

Reordering Leaves Using a Valid Order

1. Create and view a phylogenetic tree.

```
b = [1 2; 3 4; 5 6; 7 8; 9 10];
tree = phytree(b)
   Phylogenetic tree object with 6 leaves (5 branches)
view(tree)
```

2. Reorder the leaves on the phylogenetic tree, and then view the reordered tree.

```
treeReordered = reorder(tree, [5, 6, 3, 4, 1, 2])
view(treeReordered)
```

Finding Best Approximate Order When Using an Invalid Order

1. Create a phylogenetic tree by reading a Newick-formatted tree file (ASCII text file).

```
tree = phytreeread('pf00002.tree')
    Phylogenetic tree object with 33 leaves (32 branches)
```

2. Create a row vector of the leaf names in alphabetical order.

```
[dummy,order] = sort(get(tree,'LeafNames'));
```

3 Reorder the phylogenetic tree to match as closely as possible the row vector of alphabetically ordered leaf names, without dividing the clades or having crossing branches.

```
treeReordered = reorder(tree,order,'approximate',true)
    Phylogenetic tree object with 33 leaves (32 branches)
```

4 View the original and the reordered phylogenetic trees.

```
view(tree)
view(treeReordered)
```

Reordering Leaves to Match Leaf Order in Another Phylogenetic Tree

1 Create a phylogenetic tree by reading sequence data from a FASTA file, calculating the pair-wise distances between sequences, and then using the neighbor-joining method.

```
seqs = fastaread('pf00002.fa')

seqs =

33x1 struct array with fields:
    Header
    Sequence

dist = seqpdist(seqs,'method','jukes-cantor','indels','pair');
NJtree = seqneighjoin(dist,'equivar',seqs)
    Phylogenetic tree object with 33 leaves (32 branches)
```

2 Create another phylogenetic tree from the same sequence data and pair-wise distances between sequences, using the single linkage method.

```
HCtree = seqlinkage(dist,'single',seqs)
    Phylogenetic tree object with 33 leaves (32 branches)
```

3 Use the optimal leaf-ordering calculation to reorder the leaves in `HCtree` such that it matches the order of leaves in `NJtree` as closely as possible, without dividing the clades or having crossing branches.

```
HCtree_reordered = reorder(HCtree,NJtree)
    Phylogenetic tree object with 33 leaves (32 branches)
```

4 View the reordered phylogenetic tree and the tree used to reorder it.

```
view(HCtree_reordered)
view(NJtree)
```

See Also

Bioinformatics Toolbox function: `phytree` (object constructor)

Bioinformatics Toolbox object: `phytree object`

Bioinformatics Toolbox methods of a phytree object: `get`, `getbyname`, `prune`

Purpose

Change root of phylogenetic tree

Syntax

```
Tree2 = reroot(Tree1)
Tree2 = reroot(Tree1, Node)
Tree2 = reroot(Tree1, Node, Distance)
```

Arguments

Tree1	Phylogenetic tree (`phytree` object) created with the function `phytree`.
Node	Node index returned by the phytree object method `getbyname`.
Distance	Distance from the reference branch.

Description

`Tree2 = reroot(Tree1)` changes the root of a phylogenetic tree (*Tree1*) using a midpoint method. The midpoint is the location where the mean values of the branch lengths, on either side of the tree, are equalized. The original root is deleted from the tree.

`Tree2 = reroot(Tree1, Node)` changes the root of a phylogenetic tree (*Tree1*) to a branch node using the node index (*Node*). The new root is placed at half the distance between the branch node and its parent.

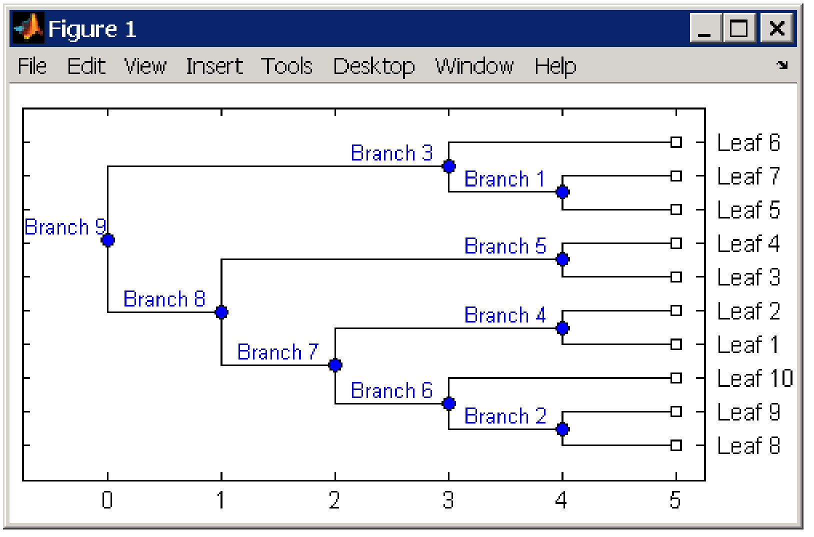
`Tree2 = reroot(Tree1, Node, Distance)` changes the root of a phylogenetic tree (*Tree1*) to a new root at a given distance (*Distance*) from the reference branch node (*Node*) toward the original root of the tree. Note: The new branch representing the root in the new tree (`Tree2`) is labeled `'Root'`.

Examples

1 Create an ultrametric tree.

```
tr_1 = phytree([5 7;8 9;6 11; 1 2;3 4;10 12;...
                14 16; 15 17;13 18])
plot(tr_1,'branchlabels',true)
```

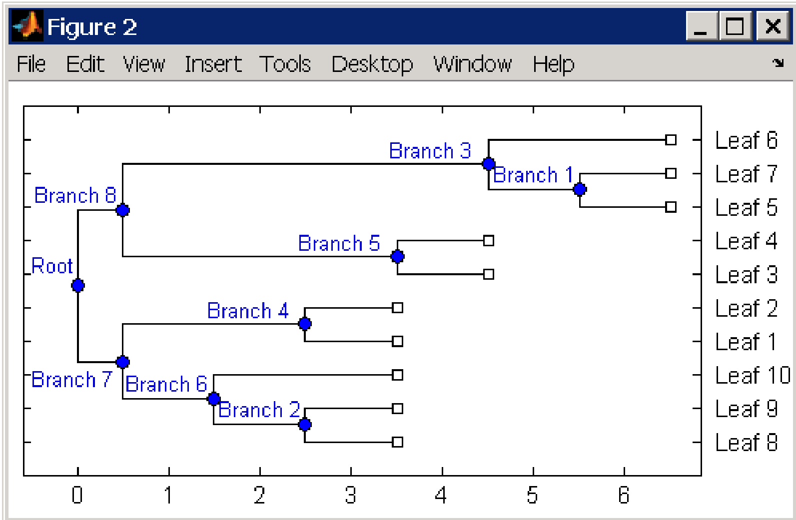
MATLAB draws a figure with the phylogenetic tree.



2 Place the root at 'Branch 7'.

```
sel = getbyname(tr_1,'Branch 7');
tr_2 =  reroot(tr_1,sel)
plot(tr_2,'branchlabels',true)
```

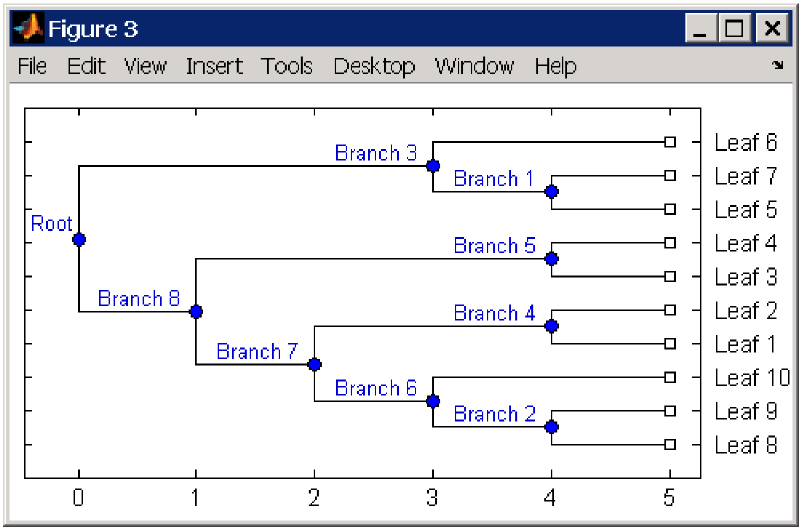
MATLAB draws a tree with the root moved to the center of branch 7.



3 Move the root to a branch that makes the tree as ultrametric as possible.

```
tr_3 = reroot(tr_2)
plot(tr_3,'branchlabels',true)
```

MATLAB draws the new tree with the root moved from the center of branch 7 to branch 8.



See Also

Bioinformatics Toolbox

- functions — `phytree` (object constructor), `seqneighjoin`
- `phytree` object methods — `get`, `getbyname`, `prune`, `select`

Purpose Select tree branches and leaves in phytree object

Syntax

```
S = select(Tree, N)
[S, Selleaves, Selbranches] = select(...)
select(..., 'PropertyName', PropertyValue,...)
select(..., 'Reference', ReferenceValue)
select(..., 'Criteria', CriteriaValue)
select(..., 'Threshold', ThresholdValue)
select(..., 'Exclude', ExcludeValue),
select(..., 'Propagate', PropagateValue)
```

Arguments

Tree	Phylogenetic tree (phytree object) created with the function phytree.
N	Number of closest nodes to the root node.
ReferenceValue	Property to select a reference point for measuring distance.
CriteriaValue	Property to select a criteria for measuring distance.
ThresholdValue	Property to select a distance value. Nodes with distances below this value are selected.
ExcludeValue	Property to remove (exclude) branch or leaf nodes from the output. Enter 'none', 'branchs', or 'leaves'. The default value is 'none'.
PropagateValue	Property to select propagating nodes toward the leaves or the root.

Description *S* = select(*Tree*, *N*) returns a logical vector (*S*) of size [NumNodes x 1] indicating the *N* closest nodes to the root node of a phytree object (Tree) where NumNodes = NumLeaves + NumBranches. The first criterion select uses is branch levels, then patristic distance (also known as tree distance). By default, `select` uses `inf` as the value of `N`, and `select(*Tree*)` returns a vector with values of `true`.

`[*S*, *Selleaves*, *Selbranches*] = select(...)` returns two additional logical vectors, one for the selected leaves and one for the selected branches.

`select(..., '*PropertyName*', *PropertyValue*,...)` defines optional properties using property name/value pairs.

`select(..., 'Reference', *ReferenceValue*)` changes the reference point(s) to measure the closeness. `Reference` can be the root (default) or leaves. When using leaves, a node can have multiple distances to its descendant leaves (nonultrametric tree). If this the case, `select` considers the minimum distance to any descendant leaf.

`select(..., 'Criteria', *CriteriaValue*)` changes the criteria `select` uses to measure closeness. If `C = 'levels'` (default), the first criterion is branch levels and then patristic distance. If `C = 'distance'`, the first criterion is patristic distance and then branch levels.

`select(..., 'Threshold', *ThresholdValue*)` selects all the nodes where closeness is less than or equal to the threshold value (`*ThresholdValue*`). Notice, you can also use either of the properties `'criteria'` or `'reference'`, if `N` is not specified, then `N = infF`; otherwise you can limit the number of selected nodes by `N`.

`select(..., 'Exclude', *ExcludeValue*)`, when `*ExcludeValue* = 'branches'`, sets a postfilter that excludes all the branch nodes from `*S*`, or when `*ExcludeValue* = 'leaves'`, all the leaf nodes. The default is `'none'`.

`select(..., 'Propagate', *PropagateValue*)` activates a postfunctionality that propagates the selected nodes to the leaves when `P=='toleaves'` or toward the root finding a common ancestor when `P == 'toroot'`. The default value is `'none'`. `P` may also be `'both'`. The `'Propagate'` property acts after the `'Exclude'` property.

Examples

```
% Load a phylogenetic tree created from a protein family:
tr = phytreeread('pf00002.tree');

% To find close products for a given protein (e.g. vips_human):
ind = getbyname(tr,'vips_human');
[sel,sel_leaves] = select(tr,'criteria','distance',...
                          'threshold',0.6,'reference',ind);
view(tr,sel_leaves)

% To find potential outliers in the tree, use
[sel,sel_leaves] = select(tr,'criteria','distance',...
                             'threshold',.3,...
                             'reference','leaves',...
                             'exclude','leaves',...
                             'propagate','toleaves');
view(tr,~sel_leaves)
```

See Also

Bioinformatics Toolbox

- functions — phytree (object constructor), phytreetool
- phytree object methods — get, pdist, prune

shortestpath (biograph)

Purpose

Solve shortest path problem in biograph object

Syntax

```
[dist, path, pred] = shortestpath(BGObj, S)
[dist, path, pred] = shortestpath(BGObj, S, T)
[...] = shortestpath(..., 'Directed', DirectedValue, ...)
[...] = shortestpath(..., 'Method', MethodValue, ...)
[...] = shortestpath(..., 'Weights', WeightsValue, ...)
```

Arguments

BGObj	biograph object created by `biograph` (object constructor).
S	Node in graph represented by an N-by-N adjacency matrix extracted from a biograph object, *BGObj*.
T	Node in graph represented by an N-by-N adjacency matrix extracted from a biograph object, *BGObj*.
DirectedValue	Property that indicates whether the graph represented by the N-by-N adjacency matrix extracted from a biograph object, *BGObj*, is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.

MethodValue String that specifies the algorithm used to find the shortest path. Choices are:

- 'Bellman-Ford' — Assumes weights of the edges to be nonzero entries in the N-by-N adjacency matrix. Time complexity is O(N*E), where N and E are the number of nodes and edges respectively.
- 'BFS' — Breadth-first search. Assumes all weights to be equal, and nonzero entries in the N-by-N adjacency matrix to represent edges. Time complexity is O(N+E), where N and E are the number of nodes and edges respectively.
- 'Acyclic' — Assumes the graph represented by the N-by-N adjacency matrix extracted from a biograph object, *BGObj*, to be a directed acyclic graph and that weights of the edges are nonzero entries in the N-by-N adjacency matrix. Time complexity is O(N+E), where N and E are the number of nodes and edges respectively.
- 'Dijkstra' — Default algorithm. Assumes weights of the edges to be positive values in the N-by-N adjacency matrix. Time complexity is O(log(N)*E), where N and E are the number of nodes and edges respectively.

WeightsValue Column vector that specifies custom weights for the edges in the N-by-N adjacency matrix extracted from a biograph object, *BGObj*. It must have one entry for every nonzero value (edge) in the N-by-N adjacency matrix. The order of the custom weights in the vector must match the order of the nonzero values in the N-by-N adjacency matrix when it is traversed column-wise. This property lets you use zero-valued weights. By default, shortestpaths gets weight information from the nonzero entries in the N-by-N adjacency matrix.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

`[dist, path, pred] = shortestpath(BGObj, S)` determines the single-source shortest paths from node `S` to all other nodes in the graph represented by an N-by-N adjacency matrix extracted from a biograph object, `BGObj`. Weights of the edges are all nonzero entries in the N-by-N adjacency matrix. `dist` are the `N` distances from the source to every node (using `Inf`s for nonreachable nodes and `0` for the source node). `path` contains the winning paths to every node. `pred` contains the predecessor nodes of the winning paths.

`[dist, path, pred] = shortestpath(BGObj, S, T)` determines the single source-single destination shortest path from node `S` to node `T`.

`[...] = shortestpath(..., 'PropertyName', PropertyValue, ...)` calls `shortestpath` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[...] = shortestpath(..., 'Directed', DirectedValue, ...)` indicates whether the graph represented by the N-by-N adjacency matrix extracted from a biograph object, `BGObj`, is directed or undirected. Set `DirectedValue` to `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.

`[...] = shortestpath(..., 'Method', MethodValue, ...)` lets you specify the algorithm used to find the shortest path. Choices are:

- `'Bellman-Ford'` — Assumes weights of the edges to be nonzero entries in the N-by-N adjacency matrix. Time complexity is `O(N*E)`, where `N` and `E` are the number of nodes and edges respectively.

- `'BFS'` — Breadth-first search. Assumes all weights to be equal, and nonzero entries in the N-by-N adjacency matrix to represent edges. Time complexity is `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively.
- `'Acyclic'` — Assumes the graph represented by the N-by-N adjacency matrix extracted from a biograph object, *`BGObj`*, to be a directed acyclic graph and that weights of the edges are nonzero entries in the N-by-N adjacency matrix. Time complexity is `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively.
- `'Dijkstra'` — Default algorithm. Assumes weights of the edges to be positive values in the N-by-N adjacency matrix. Time complexity is `O(log(N)*E)`, where `N` and `E` are the number of nodes and edges respectively.

`[...] = shortestpath(..., 'Weights', WeightsValue, ...)` lets you specify custom weights for the edges. *`WeightsValue`* is a column vector having one entry for every nonzero value (edge) in the N-by-N adjacency matrix extracted from a biograph object, *`BGObj`*. The order of the custom weights in the vector must match the order of the nonzero values in the N-by-N adjacency matrix when it is traversed column-wise. This property lets you use zero-valued weights. By default, `shortestpath` gets weight information from the nonzero entries in the N-by-N adjacency matrix.

References

[1] Dijkstra, E.W. (1959). A note on two problems in connexion with graphs. Numerische Mathematik *1*, 269-271.

[2] Bellman, R. (1958). On a Routing Problem. Quarterly of Applied Mathematics *16(1)*, 87-90.

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphshortestpath`

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `topoorder`, `traverse`

Purpose

Extract phylogenetic subtree

Syntax

Tree2 = subtree(*Tree1*, *Nodes*)

Description

Tree2 = subtree(*Tree1*, *Nodes*) extracts a new subtree (*Tree2*) where the new root is the first common ancestor of the *Nodes* vector from *Tree1*. Nodes in the tree are indexed as [1:NUMLEAVES] for the leaves and as [NUMLEAVES+1:NUMLEAVES+NUMBRANCHES] for the branches. Nodes can also be a logical array of following sizes [NUMLEAVES+NUMBRANCHES x 1], [NUMLEAVES x 1] or [NUMBRANCHES x 1].

Examples

1 Load a phylogenetic tree created from a protein family.

```
tr = phytreeread('pf00002.tree')
```

2 Get the subtree that contains the VIPS and CGRR human proteins.

```
sel = getbyname(tr,{'vips_human','cgrr_human'});
sel = any(sel,2);
tr =  subtree(tr,sel)
view(tr);
```

See Also

Bioinformatics Toolbox

- functions — phytree (object constructor)
- phytree object methods — get, getbyname, prune, select

topoorder (biograph)

Purpose

Perform topological sort of directed acyclic graph extracted from biograph object

Syntax

```
order = topoorder(BGObj)
```

Arguments

BGObj	biograph object created by `biograph` (object constructor).

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the Bioinformatics Toolbox documentation.

---

order = `topoorder(`*BGObj*`)` returns an index vector with the order of the nodes sorted topologically. In topological order, an edge can exist between a source node `u` and a destination node `v`, if and only if `u` appears before `v` in the vector *order*. *BGObj* is a biograph object from which an N-by-N adjacency matrix is extracted and represents a directed acyclic graph (DAG). In the N-by-N sparse matrix, all nonzero entries indicate the presence of an edge.

References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphtopoorder`

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `traverse`

Purpose

Traverse biograph object by following adjacent nodes

Syntax

```
[disc, pred, closed] = traverse(BGObj, S)
[...] = traverse(BGObj, S, ...'Depth', DepthValue, ...)
[...] = traverse(BGObj, S, ...'Directed', DirectedValue, ...)
[...] = traverse(BGObj, S, ...'Method', MethodValue, ...)
```

Arguments

BGObj	biograph object created by `biograph` (object constructor).
S	Integer that indicates the source node in *BGObj*.
DepthValue	Integer that indicates a node in *BGObj* that specifies the depth of the search. Default is `Inf` (infinity).
DirectedValue	Property that indicates whether graph represented by an N-by-N adjacency matrix extracted from a biograph object, *BGObj* is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.
MethodValue	String that specifies the algorithm used to traverse the graph. Choices are: • `'BFS'` — Breadth-first search. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively. • `'DFS'` — Default algorithm. Depth-first search. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

Description

Tip For introductory information on graph theory functions, see “Graph Theory Functions” in the Bioinformatics Toolbox documentation.

[*disc*, *pred*, *closed*] = traverse(*BGObj*, *S*) traverses the directed graph represented by an N-by-N adjacency matrix extracted from a biograph object, *BGObj*, starting from the node indicated by integer S. In the N-by-N sparse matrix, all nonzero entries indicate the presence of an edge. *disc* is a vector of node indices in the order in which they are discovered. *pred* is a vector of predecessor node indices (listed in the order of the node indices) of the resulting spanning tree. *closed* is a vector of node indices in the order in which they are closed.

[...] = traverse(*BGObj*, *S*, ...'*PropertyName*', *PropertyValue*, ...) calls traverse with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

[...] = traverse(*BGObj*, *S*, ...'Depth', *DepthValue*, ...) specifies the depth of the search. *DepthValue* is an integer indicating a node in the graph represented by the N-by-N adjacency matrix extracted from a biograph object, *BGObj*. Default is Inf (infinity).

[...] = traverse(*BGObj*, *S*, ...'Directed', *DirectedValue*, ...) indicates whether the graph represented by the N-by-N adjacency matrix extracted from a biograph object, *BGObj* is directed or undirected. Set *DirectedValue* to false for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is true.

[...] = traverse(*BGObj*, *S*, ...'Method', *MethodValue*, ...) lets you specify the algorithm used to traverse the graph represented by the N-by-N adjacency matrix extracted from a biograph object, *BGObj*. Choices are:

- 'BFS' — Breadth-first search. Time complexity is O(N+E), where N and E are number of nodes and edges respectively.
- 'DFS' — Default algorithm. Depth-first search. Time complexity is O(N+E), where N and E are number of nodes and edges respectively.

References

[1] Sedgewick, R., (2002). Algorithms in C++, Part 5 Graph Algorithms (Addison-Wesley).

[2] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphtraverse`

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`

view (biograph)

Purpose

Draw figure from biograph object

Syntax

```
view(BGobj)
BGobjHandle = view(BGobj)
```

Arguments

BGobj	Biograph object created with the function `biograph`.

Description

`view(`*BGobj*`)` opens a figure window and draws a graph represented by a biograph object (*BGobj*). When the biograph object is already drawn in the figure window, this function only updates the graph properties.

BGobjHandle `= view(`*BGobj*`)` returns a handle to a deep copy of the biograph object (`BGobj`) in the figure window. When updating an existing figure, you can use the returned handle to change object properties programmatically or from the command line. When you close the figure window, the handle is no longer valid. The original biograph object (*BGobj*) is left unchanged.

Examples

1 Create a biograph object.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
bg = biograph(cm)
```

2 Render the biograph object into a Handles Graphic figure and get back a handle.

```
h = view(bg)
```

3 Change the color of all nodes and edges.

```
set(h.Nodes,'Color',[.5 .7 1])
set(h.Edges,'LineColor',[0 0 0])
```

See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

MATLAB functions: `get`, `set`

view (phytree)

Purpose

View phylogenetic tree

Syntax

```
view(Tree)
view(Tree, IntNodes)
```

Arguments

Tree	Phylogenetic tree (phytree object) created with the function phytree.
IntNodes	Nodes from the phytree object to initially display in the *Tree*.

Description

view(*Tree*) opens the Phylogenetic Tree Tool window and draws a tree from data in a phytree object (*Tree*). The significant distances between branches and nodes are in the horizontal direction. Vertical distances have no significance and are selected only for display purposes. You can access tools to edit and analyze the tree from the Phylogenetic Tree Tool menu bar or by using the left and right mouse buttons.

view(*Tree*, *IntNodes*) opens the Phylogenetic Tree Tool window with an initial selection of nodes specified by *IntNodes*. *IntNodes* can be a logical array of any of the following sizes: NumLeaves + NumBranches x 1, NumLeaves x 1, or NumBranches x 1. *IntNodes* can also be a list of indices.

Example

```
tree = phytreeread('pf00002.tree')
view(tree)
```

See Also

Bioinformatics Toolbox functions: phytree (object constructor), phytreeread, phytreetool, seqlinkage, seqneighjoin

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox method of phytree object: plot

Purpose

Calculate weights for phylogenetic tree

Syntax

`W = weights(Tree)`

Arguments

Tree	Phylogenetic tree (`phytree` object) created with the function `phytree`.

Description

`W = weights(Tree)` calculates branch proportional weights for every leaf in a tree (*Tree*) using the Thompson-Higgins-Gibson method. The distance of every segment of the tree is adjusted by dividing it by the number of leaves it contains. The sequence weights are the result of normalizing to unity the new patristic distances between every leaf and the root.

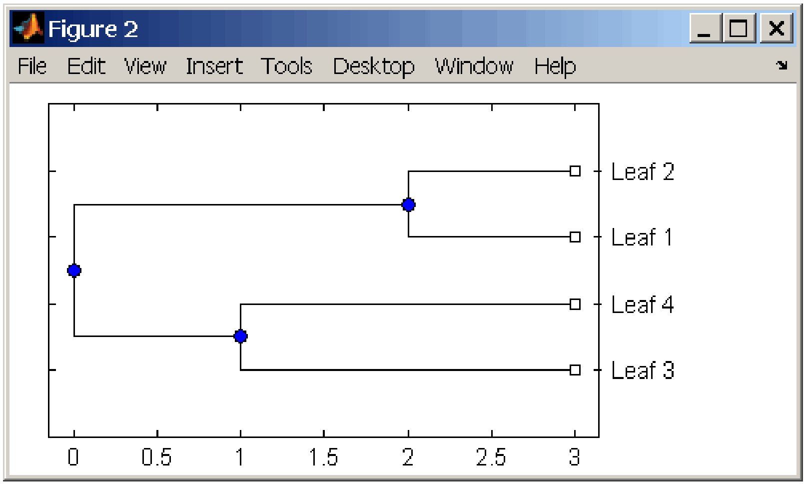
Examples

1 Create an ultrametric tree with specified branch distances.

```
bd = [1 2 3]';
tr_1 = phytree([1 2;3 4;5 6],bd)
```

2 View the tree.

```
view(tr_1)
```



3 Display the calculated weights.

```
weights(tr_1)

ans =

    1.0000
    1.0000
    0.8000
    0.8000
```

References

[1] Thompson JD, Higgins DG, Gibson TJ (1994), "CLUSTAL W: Improving the sensitivity of progressive multiple sequence alignment through sequence weighting, position-specific gap penalties and weight matrix choice," Nucleic Acids Research, 22(22):4673-4680.

[2] Henikoff S, Henikoff JG (1994), "Position-based sequence weights," Journal Molecular Biology, 243(4):574-578.

See Also

Bioinformatics Toolbox

- functions — `multialign`, `phytree` (object constructor), `profalign`, `seqlinkage`

Objects — Alphabetical List

Purpose

Data structure containing generic interconnected data used to implement directed graph

Description

A biograph object is a data structure containing generic interconnected data used to implement a directed graph. Nodes represent proteins, genes, or any other biological entity, and edges represent interactions, dependences, or any other relationship between the nodes. A biograph object also stores information, such as color properties and text label characteristics, used to create a 2-D visualization of the graph.

You create a biograph object using the object constructor function `biograph`. You can view a graphical representation of a biograph object using the `view` method.

Method Summary

Following are methods of a biograph object:

allshortestpaths (biograph)	Find all shortest paths in biograph object
conncomp (biograph)	Find strongly or weakly connected components in biograph object
dolayout (biograph)	Calculate node positions and edge trajectories
getancestors (biograph)	Find ancestors in biograph object
getdescendants (biograph)	Find descendants in biograph object
getedgesbynodeid (biograph)	Get handles to edges in biograph object
getmatrix (biograph)	Get connection matrix from biograph object
getnodesbyid (biograph)	Get handles to nodes
getrelatives (biograph)	Find relatives in biograph object
isdag (biograph)	Test for cycles in biograph object

isomorphism (biograph)	Find isomorphism between two biograph objects
isspantree (biograph)	Determine if tree created from biograph object is spanning tree
maxflow (biograph)	Calculate maximum flow and minimum cut in biograph object
minspantree (biograph)	Find minimal spanning tree in biograph object
shortestpath (biograph)	Solve shortest path problem in biograph object
topoorder (biograph)	Perform topological sort of directed acyclic graph extracted from biograph object
traverse (biograph)	Traverse biograph object by following adjacent nodes
view (biograph)	Draw figure from biograph object

Following are methods of a node object:

getancestors (biograph)	Find ancestors in biograph object
getdescendants (biograph)	Find descendants in biograph object
getrelatives (biograph)	Find relatives in biograph object

Property Summary

A biograph object contains two objects, node objects and edge objects, that have their own properties. For a list of the properties of node objects and edge objects, see the following tables.

Properties of a Biograph Object

Property	Description
`ID`	String to identify the biograph object. Default is `''`. (This information is for bookkeeping purposes only.)
`Label`	String to label the biograph object. Default is `''`. (This information is for bookkeeping purposes only.)
`Description`	String that describes the biograph object. Default is `''`. (This information is for bookkeeping purposes only.)
`LayoutType`	String that specifies the algorithm for the layout engine. Choices are: • `'hierarchical'` (default) • `'equilibrium'` • `'radial'`
`EdgeType`	String that specifies how edges display. Choices are: • `'straight'` • `'curved'` (default) • `'segmented'` **Note** Curved or segmented edges occur only when necessary to avoid obstruction by nodes. Biograph objects with `LayoutType` equal to `'equilibrium'` or `'radial'` cannot produce curved or segmented edges.
`Scale`	Positive number that post-scales the node coordinates. Default is `1`.

Property	Description
LayoutScale	Positive number that scales the size of the nodes before calling the layout engine. Default is 1.
EdgeTextColor	Three-element numeric vector of RGB values. Default is [0, 0, 0], which defines black.
EdgeFontSize	Positive number that sets the size of the edge font in points. Default is 8.
ShowArrows	Controls the display of arrows with the edges. Choices are 'on' (default) or 'off'.
ArrowSize	Positive number that sets the size of the arrows in points. Default is 8.
ShowWeights	Controls the display of text indicating the weight of the edges. Choices are 'on' (default) or 'off'.
ShowTextInNodes	String that specifies the node property used to label nodes when you display a biograph object using the view method. Choices are: • 'Label' — Uses the Label property of the node object (default). • 'ID' — Uses the ID property of the node object. • 'None'

Property	Description
NodeAutoSize	Controls precalculating the node size before calling the layout engine. Choices are 'on' (default) or 'off'.
NodeCallback	User-defined callback for all nodes. Enter the name of a function, a function handle, or a cell array with multiple function handles. After using the view function to display the biograph object in the Biograph Viewer, you can double-click a node to activate the first callback, or right-click and select a callback to activate. Default is the anonymous function, @(node) inspect(node), which displays the Property Inspector dialog box.
EdgeCallback	User-defined callback for all edges. Enter the name of a function, a function handle, or a cell array with multiple function handles. After using the view function to display the biograph object in the Biograph Viewer, you can double-click an edge to activate the first callback, or right-click and select a callback to activate. Default is the anonymous function, @(edge) inspect(edge), which displays the Property Inspector dialog box.
CustomNodeDrawFcn	Function handle to customized function to draw nodes. Default is [].

Property	Description
Nodes	Read-only column vector with handles to node objects of a biograph object. The size of the vector is the number of nodes. For properties of node objects, see Properties of a Node Object on page 5-7.
Edges	Read-only column vector with handles to edge objects of a biograph object. The size of vector is the number of edges. For properties of edge objects, see Properties of an Edge Object on page 5-9.

Properties of a Node Object

Property	Description
`ID`	Read-only string defined when the biograph object is created, either by the *`NodeIDs`* input argument or internally by the `biograph` constructor function. Each node object's `ID` is unique and used internally to identify the node.
`Label`	String for labeling a node when you display a biograph object using the `view` method. Default is the `ID` property of the node object.
`Description`	String that describes the node. Default is `''`. (This information is for bookkeeping purposes only.)
`Position`	Two-element numeric vector of *x*- and *y*-coordinates, for example, `[150, 150]`. If you do not specify this property, default is initially `[]`, then when the layout algorithms are executed, it becomes a two-element numeric vector of *x*- and *y*-coordinates computed by the layout engine.

Property	Description
Shape	String that specifies the shape of the nodes. Choices are: • 'box'(default) • 'ellipse' • 'circle' • 'rectangle' • 'diamond' • 'trapezium' • 'invtrapezium' • 'house' • 'inverse' • 'parallelogram'
Size	Two-element numeric vector calculated before calling the layout engine using the actual font size and shape of the node. Default is [10, 10].
Color	Three-element numeric vector of RGB values that specifies the fill color of the node. Default is [1, 1, 0.7], which defines yellow.
LineWidth	Positive number. Default is 1.
LineColor	Three-element numeric vector of RGB values that specifies the outline color of the node. Default is [0.3, 0.3, 1], which defines blue.
FontSize	Positive number that sets the size of the node font in points. Default is 8.

Property	Description
TextColor	Three-element numeric vector of RGB values that specifies the color of the node labels. Default is [0, 0, 0], which defines black.
UserData	Miscellaneous, user-defined data that you want to associate with the node. The node does not use this property, but you can access and specify it using the get and set functions. Default is [].

Properties of an Edge Object

Property	Description
ID	Read-only string defined when the biograph object is created, internally by the biograph constructor function. Each edge object's ID is unique and used internally to identify the edge.
Label	String for labeling an edge when you display a biograph object using the view method. Default is the ID property of the edge object.
Description	String that describes the edge. Default is ''. (This information is for bookkeeping purposes only.)
Weight	Value that represents the weight (cost, distance, length, or capacity) associated with the edge. Default is 1.
LineWidth	Positive number. Default is 1.
LineColor	Three-element numeric vector of RGB values that specifies the color of the edge. Default is [0.5, 0.5, 0.5], which defines gray.
UserData	Miscellaneous, user-defined data that you want to associate with the edge. The edge does not use this property, but you can access and specify it using the get and set functions. Default is [].

Examples

Accessing Properties of a Biograph Object

You can access properties of a biograph object, *BGobj*, by using either of the following syntaxes:

`PropertyValue = get(BGobj, 'PropertyName')`

`PropertyValue = BGobj.PropertyName`

Accessing Allowed Values of Biograph Object Properties

You can access allowed values for any property that has a finite set of choices by using the following syntax:

`set(BGobj, 'PropertyName')`

Specifying Properties of a Biograph Object

You can specify properties of a biograph object, *BGobj*, by using any of the following syntaxes:

`set(BGobj, 'PropertyName', PropertyValue)`

`BGobj.PropertyName = PropertyValue`

See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getmatrix`, `getnodesbyid`, `getrelatives`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`, `traverse`, `view`

MATLAB functions: `get`, `set`

Purpose

Data structure containing Gene Ontology (GO) information

Description

A geneont object is a data structure containing Gene Ontology information. Gene Ontology terms can be explored and traversed through "is_a" and "part_of" relationships.

Method Summary

Following are methods of a geneont object:

getancestors (geneont)	Numeric IDs for ancestors of Gene Ontology term
getdescendants (geneont)	Numeric IDs for descendants of Gene Ontology term
getmatrix (geneont)	Convert geneont object into relationship matrix
getrelatives (geneont)	Numeric IDs for relatives of Gene Ontology term

Property Summary

Properties of a geneont Object

Property	Description
`default_namespace`	Read-only string containing the namespace to which terms are assigned.
`format_version`	Read-only string containing the version of the encoding of the OBO flat format file.
`date`	Read-only string containing the date the OBO file was last updated.
`Terms`	Read-only column vector with handles to term objects of a geneont object. For properties of term objects, see Properties of Terms Objects on page 5-12.

Properties of Terms Objects

Property	Description
id	Numeric value that corresponds to the GO ID of the GO term. **Tip** You can use the num2goid function to convert id to a GO ID string.
name	String representing the name of the GO term.
ontology	String limited to 'molecular function', 'biological process', or 'cellular component'.
definition	String that defines the GO term.
synonym	Numeric array containing GO IDs of GO terms that are synonyms of this GO term.
is_a	Numeric array containing GO IDs of GO terms that have an "is_a" relationship with this GO term.
part_of	Numeric array containing GO IDs that of GO terms that have a "part_of" relationship with this GO term.
obsolete	Boolean value that indicates if the GO term is obsolete (1) or not obsolete (0).

See Also

Bioinformatics Toolbox functions: geneont (object constructor), goannotread, num2goid

Bioinformatics Toolbox methods of geneont object: getancestors, getdescendants, getmatrix, getrelatives

Purpose

Data structure containing phylogenetic tree

Description

A phytree object is a data structure containing a phylogenetic tree. Phylogenetic trees are binary rooted trees, which means that each branch is the parent of two other branches, two leaves, or one branch and one leaf. A phytree object can be ultrametric or nonultrametric.

Method Summary

Following are methods of a phytree object:

get (phytree)	Information about phylogenetic tree object
getbyname (phytree)	Branches and leaves from phytree object
getcanonical (phytree)	Calculate canonical form of phylogenetic tree
getmatrix (phytree)	Convert phytree object into relationship matrix
getnewickstr (phytree)	Create Newick-formatted string
pdist (phytree)	Calculate pair-wise patristic distances in phytree object
plot (phytree)	Draw phylogenetic tree
prune (phytree)	Remove branch nodes from phylogenetic tree
reorder (phytree)	Reorder leaves of phylogenetic tree
reroot (phytree)	Change root of phylogenetic tree
select (phytree)	Select tree branches and leaves in phytree object
subtree (phytree)	Extract phylogenetic subtree

view (phytree)	View phylogenetic tree
weights (phytree)	Calculate weights for phylogenetic tree

Property Summary

Note You cannot modify these properties directly. You can access these properties using the `get` method.

Property	Description
`NumLeaves`	Number of leaves
`NumBranches`	Number of branches
`NumNodes`	Number of nodes (`NumLeaves + NumBranches`)
`Pointers`	Branch to leaf/branch connectivity list
`Distances`	Edge length for every leaf/branch
`LeafNames`	Names of the leaves
`BranchNames`	Names of the branches
`NodeNames`	Names of all the nodes

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreeread`, `phytreetool`, `phytreewrite`, `seqlinkage`, `seqneighjoin`, `seqpdist`

Bioinformatics Toolbox methods of phytree object: `get`, `getbyname`, `getcanonical`, `getmatrix`, `getnewickstr`, `pdist`, `plot`, `prune`, `reroot`, `select`, `subtree`, `view`, `weights`

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