The Structural Representation of Proximity Matrices With MATLAB

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Part I

(Multi- and Uni-dimensional) City-Block Scaling

Chapter 1

Linear Unidimensional Scaling

The task of linear unidimensional scaling (LUS) can be characterized as a specific data analysis problem: given a set of n objects, $S = \{O_1, ..., O_n\}$, and an $n \times n$ symmetric proximity matrix $\mathbf{P} = \{p_{ij}\}$, arrange the objects along a single dimension such that the induced $n(n-1)/2$ interpoint distances between the objects reflect the proximities in $\mathbf{P}$. The term "proximity" refers to any symmetric numerical measure of relationship between each object pair ($p_{ij} = p_{ji}$ for $1 \leq i, j \leq n$) and for which all self-proximities are considered irrelevant and set equal to zero ($p_{ii} = 0$ for $1 \leq i \leq n$). As a technical convenience, proximities are assumed nonnegative and are given a dissimilarity interpretation, so that large proximities refer to dissimilar objects.

As a starting point to be developed exclusively in this first chapter, we consider the most common formalization of measuring how close the interpoint distances are to the given proximities by the sum of squared discrepancies. Specifically, we wish to find the n coordinates, $x_1, x_2, \ldots, x_n$, such that the least-squares (or L_2) criterion

$$\sum_{i<j}(p_{ij} - |x_j - x_i|)^2 \tag{1.1}$$

is minimized. Although there is some arbitrariness in the selection of this measure of goodness-of-fit for metric scaling, the choice is traditional and has been discussed in some detail in the literature by Guttman (1968), Defays (1978), de Leeuw and Heiser (1977), and Hubert and Arabie (1986), among others. In the various sections that follow, we will develop a particular heuristic strategy for the minimization of (1.1) based on the iterative use of a quadratic assignment improvement technique. Other methods are possible but will not be explicitly discussed here; the reader is referred to Hubert, Arabie, and Meulman (2002) for a comparison among several optimization alternatives for the basic LUS task.

In addition to developing the combinatorial optimization task of actually identifying a best unidimensional scaling, Section 1.3 introduces two additional problems within the LUS context: (a) the confirmatory fitting of a unidimensional scale (through coordinate estimation) based on a fixed (and given) object ordering; (b) the extension to nonmetric unidimensional scaling incorporating an additional optimal monotonic transformation of the proximities. Both of these optimization tasks are formulated through the L_2 norm and carried out through applications of what is called the Dykstra-Kaczmarz method of solving linear (in)equality constrained least-squares tasks. The latter strategy is reviewed briefly in a short addendum (in Section 1.4) to this chapter.

1.1 LUS in the L_2 Norm

As a reformulation of the L_2 unidimensional scaling task that will prove crucial as a point of departure in our development of a computational routine, the optimization suggested by (1.1) can be subdivided into two separate problems to be solved simultaneously: find a set of n numbers, $x_1 \leq x_2 \leq \cdots \leq x_n$, *and* a permutation on the first n integers, $\rho(\cdot) \equiv \rho$, for which

$$\sum_{i<j} (p_{\rho(i)\rho(j)} - (x_j - x_i))^2 \tag{1.2}$$

is minimized. Thus, a set of locations (coordinates) is defined along a continuum as represented in ascending order by the sequence $x_1, x_2, \ldots, x_n$; the n objects are allocated to these locations by the permutation ρ, so object $O_{\rho(i)}$ is placed at location i. Without loss of generality we will impose the one additional constraint that $\sum_i x_i = 0$, i.e., any set of values, $x_1, x_2, \ldots, x_n$, can be replaced by $x_1 - \bar{x}, x_2 - \bar{x}, \ldots, x_n - \bar{x}$, where $\bar{x} = (1/n)\sum_i x_i$, without altering the value of (1.1) or (1.2). Formally, if ρ^* and $x_1^* \leq x_2^* \leq \cdots \leq x_n^*$ define a global minimum of (1.2), and Ω denotes the set of all permutations of the first n integers, then

$$\sum_{i<j} (p_{\rho^*(i)\rho^*(j)} - (x_j^* - x_i^*))^2 =$$

$$\min[\sum_{i<j} (p_{\rho(i)\rho(j)} - (x_j - x_i))^2 \mid \rho \in \Omega;\ x_1 \leq \cdots \leq x_n;\ \sum_i x_i = 0].$$

The measure of loss in (1.2) can be reduced algebraically:

$$\sum_{i<j} p_{ij}^2 + n(\sum_i x_i^2 - 2\sum_i x_i t_i^{(\rho)}), \tag{1.3}$$

subject to the constraints that $x_1 \leq \cdots \leq x_n$ and $\sum_i x_i = 0$, and letting

$$t_i^{(\rho)} = (u_i^{(\rho)} - v_i^{(\rho)})/n,$$

where

$$u_i^{(\rho)} = \sum_{j=1}^{i-1} p_{\rho(i)\rho(j)} \text{ for } i \geq 2;$$

$$v_i^{(\rho)} = \sum_{j=i+1}^{n} p_{\rho(i)\rho(j)} \text{ for } i < n,$$

and

$$u_1^{(\rho)} = v_n^{(\rho)} = 0.$$

In words, $u_i^{(\rho)}$ is the sum of the entries within row $\rho(i)$ of $\{p_{\rho(i)\rho(j)}\}$ from the extreme left up to the main diagonal; $v_i^{(\rho)}$ is the sum from the main diagonal to the extreme right. Or, we might rewrite (1.3) as

$$\sum_{i<j} p_{ij}^2 + n\left(\sum_i (x_i - t_i^{(\rho)})^2 - \sum_i (t_i^{(\rho)})^2\right). \tag{1.4}$$

In (1.4), the two terms $\sum_i (x_i - t_i^{(\rho)})^2$ and $\sum_i (t_i^{(\rho)})^2$ control the size of the discrepancy index since $\sum_{i<j} p_{ij}^2$ is constant for any given data matrix. Thus, to minimize the original index in (1.2), we should simultaneously minimize $\sum_i (x_i - t_i^{(\rho)})^2$ and maximize $\sum_i (t_i^{(\rho)})^2$. If the equivalent form of (1.3) is considered, our concern would be in minimizing $\sum_i x_i^2$ and maximizing $\sum_i x_i t_i^{(\rho)}$.

As noted first by Defays (1978), the minimization of (1.4) can be carried out directly by the maximization of the single term, $\sum_i (t_i^{(\rho)})^2$ (under the mild regularity condition that all off-diagonal proximities in $\mathbf{P}$ are positive and not merely nonnegative). Explicitly, if ρ^* is a permutation that maximizes $\sum_i (t_i^{(\rho)})^2$, then we can let $x_i = t_i^{(\rho^*)}$, which eliminates the term $\sum_i (x_i - t_i^{(\rho^*)})^2$ from (1.4). In short, because the order induced by $t_1^{(\rho^*)}, \ldots, t_n^{(\rho^*)}$ is consistent with the constraint $x_1 \leq x_2 \leq \cdots \leq x_n$, the minimization of (1.4) reduces to the maximization of the single term $\sum_i (t_i^{(\rho)})^2$, with the coordinate estimation completed as an automatic byproduct.

1.1.1 A Data Set for Illustrative Purposes

It is convenient to have a small numerical example available as we discuss the various optimization strategies in the unidimensional scaling context. To this end we list a data file in Table 1.1, called '`number.dat`', that contains a dissimilarity matrix taken from Shepard, Kilpatric, and Cunningham (1975). The stimulus domain is the first ten single-digits {0,1,2, ..., 9} considered as abstract concepts; the 10 × 10 proximity matrix (with an i^{th} row or column corresponding to the $i - 1$ digit) was constructed by averaging dissimilarity ratings for distinct pairs of those integers over a number of subjects and conditions. Given the various analyses of this proximity matrix that have appeared in the literature (e.g., see Hubert, Arabie, and Meulman, 2001), the data reflect two types of very regular patterning based on absolute digit magnitude and the structural characteristics of the digits (e.g., the powers of 2 or of 3, the salience of the two additive/multiplicative identities [0/1], oddness/evenness). These data will be relied on to provide concrete numerical illustrations of the various MATLAB functions we introduce, and will be loaded as a proximity matrix (and importantly, as one that is symmetric and has zero values along the main diagonal) in the MATLAB environment by the command `'load number.dat'`. As we will see in the various applications, the dominant single unidimensional scale found for these data is most consistent with digit magnitude.

Table 1.1: The number.dat data file from Shepard, Kilpatric, and Cunningham (1975)

.000	.421	.584	.709	.684	.804	.788	.909	.821	.850
.421	.000	.284	.346	.646	.588	.758	.630	.791	.625
.584	.284	.000	.354	.059	.671	.421	.796	.367	.808
.709	.346	.354	.000	.413	.429	.300	.592	.804	.263
.684	.646	.059	.413	.000	.409	.388	.742	.246	.683
.804	.588	.671	.429	.409	.000	.396	.400	.671	.592
.788	.758	.421	.300	.388	.396	.000	.417	.350	.296
.909	.630	.796	.592	.742	.400	.417	.000	.400	.459
.821	.791	.367	.804	.246	.671	.350	.400	.000	.392
.850	.625	.808	.263	.683	.592	.296	.459	.392	.000

1.2 L_2-Norm Optimization Methods

This section shows how a well-known combinatorial optimization task, called quadratic assignment, can be used iteratively for LUS in the L_2-norm. Based on the reformulation in (1.3), we concentrate on maximizing $\sum_i x_i t_i^{(\rho)}$, with iterative re-estimation of the coordinates $x_1, \ldots, x_n$. Various function implementations within MATLAB are given both for the basic quadratic assignment task as well as for how it is used for LUS.

1.2.1 Iterative Quadratic Assignment

Because of the manner in which the discrepancy index for the unidimensional scaling task can be rephrased as in (1.3) and (1.4), the two optimization subproblems to be solved simultaneously of identifying an optimal permutation and a set of coordinates can be separated:

(a) assuming that an ordering of the objects is known (and denoted, say, as ρ^0 for the moment), find those values $x_1^0 \leq \cdots \leq x_n^0$ to minimize $\sum_i (x_i^0 - t_i^{(\rho^0)})^2$. If the permutation ρ^0 produces a *monotonic* form for the matrix $\{p_{\rho^0(i)\rho^0(j)}\}$ in the sense that $t_1^{(\rho^0)} \leq t_2^{(\rho^0)} \leq \cdots \leq t_n^{(\rho^0)}$, the coordinate estimation is immediate by letting $x_i^0 = t_i^{(\rho^0)}$, in which case $\sum_i (x_i^0 - t_i^{(\rho^0)})^2$ is zero.

(b) assuming that the locations $x_1^0 \leq \cdots \leq x_n^0$ are known, find the permutation ρ^0 to maximize $\sum_i x_i t_i^{(\rho^0)}$. We note from the work of Hubert and Arabie (1986, p. 189) that any such permutation which even only locally maximizes $\sum_i x_i t_i^{(\rho^0)}$, in the sense that no adjacently placed pair of objects in ρ^0 could be interchanged to increase the index, will produce a monotonic form for the non-negative matrix $\{p_{\rho^0(i)\rho^0(j)}\}$. Also, the task of finding the permutation ρ^0 to maximize $\sum_i x_i t_i^{(\rho^0)}$ is actually a quadratic assignment (QA) task which has been discussed extensively in the literature of operations research, e.g., see Francis and White (1974), Lawler (1975), Hubert and Schultz (1976), among others. As usually defined, a

QA problem involves two $n \times n$ matrices $\mathbf{A} = \{a_{ij}\}$ and $\mathbf{B} = \{b_{ij}\}$, and we seek a permutation ρ to maximize

$$\Gamma(\rho) = \sum_{i,j} a_{\rho(i)\rho(j)} b_{ij}. \tag{1.5}$$

If we define $b_{ij} = |x_i - x_j|$ and let $a_{ij} = p_{ij}$, then

$$\Gamma(\rho) = \sum_{i,j} p_{\rho(i)\rho(j)} |x_i - x_j| = 2n \sum_i x_i t_i^{(\rho)},$$

and thus, the permutation that maximizes $\Gamma(\rho)$ also maximizes $\sum x_i t_i^{(\rho)}$.

The QA optimization task as formulated through (1.5) has an enormous literature attached to it, and the reader is referred to Pardalos and Wolkowicz (1994) for an up-to-date and comprehensive review. For current purposes and as provided in three general m-functions of the next section (`pairwiseqa.m`, `rotateqa.m`, and `insertqa.m`), one might consider the optimization of (1.5) through simple object interchange/rearrangement heuristics. Based on given matrices **A** and **B**, and beginning with some permutation (possibly chosen at random), local interchanges/rearrangements of a particular type are implemented until no improvement in the index can be made. By repeatedly initializing such a process randomly, a distribution over a set of local optima can be achieved. At least within the context of some common data analysis applications, such a distribution may be highly relevant diagnostically for explaining whatever structure might be inherent in the matrix **A**.

In a subsequent subsection below, we introduce the main m-function (`uniscalqa.m`) for unidimensional scaling based on these earlier QA optimization strategies. In effect, we begin with an equally-spaced set of fixed coordinates with their interpoint distances defining the **B** matrix of the general QA index in (1.5) and a random object permutation; a locally-optimal permutation is then identified through a collection of local interchanges/rearrangements; the coordinates are re-estimated based on this identified permutation, and the whole process repeated until no change can be made in either the identified permutation or coordinate collection.

The QA interchange/rearrangement heuristics

The three m-functions that carry out general QA interchange/rearrangement heuristics all have the same general usage syntax (note the use of three dots to denote a statement continuation in MATLAB):

```
[outperm rawindex allperms index] = pairwiseqa(prox,targ,inperm)

[outperm rawindex allperms index] = ...
                          rotateqa(prox,targ,inperm,kblock)

[outperm rawindex allperms index] = ...
                          insertqa(prox,targ,inperm,kblock)
```

pairwiseqa.m carries out an iterative QA maximization task using the pairwise interchanges of objects in the current permutation defining the row and column order of the data matrix. All possible such interchanges are generated and considered in turn, and whenever an increase in the cross-product index would result from a particular interchange, it is made immediately. The process continues until the current permutation cannot be improved upon by any such pairwise object interchange; this final locally optimal permutation is OUTPERM. The input beginning permutation is INPERM (a permutation of the first n integers); PROX is the $n \times n$ input proximity matrix and TARG is the $n \times n$ input target matrix (which are respective analogues of the matrices $\mathbf{A}$ and $\mathbf{B}$ of (1.5)); the final OUTPERM row and column permutation of PROX has the cross-product index RAWINDEX with respect to TARG. The cell array ALLPERMS contains INDEX entries corresponding to all the permutations identified in the optimization, from ALLPERMS{1} = INPERM to ALLPERMS{INDEX} = OUTPERM. (Note that within a MATLAB environment, entries of a cell array must be accessed through the curly braces, { }.) rotateqa.m carries out a similar iterative QA maximization task but now uses the rotation (or inversion) of from 2 to KBLOCK (which is less than or equal to $n - 1$) consecutive objects in the current permutation defining the row and column order of the data matrix. insertqa.m relies on the (re-)insertion of from 1 to KBLOCK consecutive objects somewhere in the permutation defining the current row and column order of the data matrix.

The MATLAB function uniscalqa.m

The MATLAB function m-file, uniscalqa.m, carries out a unidimensional scaling of a symmetric dissimilarity matrix (with a zero main diagonal) using an iterative quadratic assignment strategy. We begin with an equally-spaced target, a (random) starting permutation, and use a sequential combination of the pairwise interchange/rotation/insertion heuristics; the target matrix is re-estimated based on the identified (locally optimal) permutation. The whole process is repeated until no changes can be made in the target or the identified (locally optimal) permutation. The explicit usage syntax is

```
[outperm rawindex allperms index coord diff] = ...
                    uniscalqa(prox,targ,inperm,kblock)
```

where all terms are (mostly) present in the three QA heuristic m-functions of the previous subsection. Here, COORD gives the final coordinates achieved, and DIFF provides the attained value for the least-squares loss function. A recording of a MATLAB session using number.dat follows; note the application of the built-in MATLAB function randperm(10) to obtain a random input permutation of the first 10 digits, and the use of the utility m-function, targlin.m (and the command targlin(10)), to generate a target matrix targlinear based on an equally (and unit) spaced set of coordinates. In the output given below, semicolons are placed after the invocation of the m-functions to initially suppress the output; transposes(') are then used on the output vectors to conserve space by only using row (as opposed to column) vectors in the listing; also, to conserve space, blank lines are typically deleted in any output given throughout this chapter as well as in the chapters that follow.

```
>> load number.dat
>> targlinear = targlin(10);
>> inperm = randperm(10);
>> kblock = 2;
>> [outperm rawindex allperms index coord diff] = ...
uniscalqa(number,targlinear,inperm,kblock);
>> outperm
outperm =
     8    10     9     7     6     4     5     3     2     1
>> coord'
ans =
  Columns 1 through 6
   -0.5345   -0.4050   -0.3258   -0.1988   -0.0842    0.0566
  Columns 7 through 10
    0.1492    0.2608    0.4247    0.6570
>> diff
diff =
    1.9599
```

1.3 Confirmatory and Nonmetric LUS

In developing linear unidimensional scaling (as well as other types of) representations for a proximity matrix, it is convenient to have a general mechanism available for solving linear (in)equality constrained least-squares tasks. The two such instances discussed in this section involve (a) the confirmatory fitting of a given object order to a proximity matrix (through an m-file called `linfit.m`), and (b) the construction of an optimal monotonic transformation of a proximity matrix in relation to a given unidimensional ordering (through an m-file called `proxmon.m`). In both of these cases, we rely on what can be called the Dykstra-Kaczmarz method. An equality constrained least-squares task may be rephrased as a linear system of equations, with the later solvable through a strategy of iterative projection as attributed to Kaczmarz (1937; see Bodewig, 1956, pp. 163–164); a more general inequality constrained least-squares task can also be approached through iterative projection as developed by Dykstra (1983). The Kaczmarz and Dykstra strategies are reviewed very briefly in the chapter addendum, and implemented within the two m-files, `linfit.m` and `proxmon.m`, discussed below.

1.3.1 The confirmatory fitting of a given order using the MATLAB function linfit.m

The MATLAB m-function, `linfit.m`, fits a set of coordinates to a given proximity matrix based on some given input permutation, say, $\rho^{(0)}$. Specifically, we seek $x_1 \leq x_2 \leq \cdots \leq x_n$

such that $\sum_{i<j}(p_{\rho^0(i)\rho^0(j)} - |x_j - x_i|)^2$ is minimized (and where the permutation $\rho^{(0)}$ may not even put the matrix $\{p_{\rho^0(i)\rho^0(j)}\}$ into a monotonic form). Using the syntax

```
[fit diff coord] = linfit(prox,inperm)
```

the matrix $\{|x_j - x_i|\}$ is referred to as the fitted matrix (`FIT`); `COORD` gives the ordered coordinates; and `DIFF` is the value of the least-squares criterion. The fitted matrix is found through the Dykstra-Kaczmarz method where the equality constraints defined by distances along a continuum are imposed to find the fitted matrix, i.e., if $i < j < k$, then $|x_i - x_j| + |x_j - x_k| = |x_i - x_k|$. Once found, the actual ordered coordinates are retrieved by the usual $t_i^{(\rho^0)}$ formula used in (1.3) but computed on `FIT`.

The example below of the use of `linfit.m` fits two separate orders: the identity permutation and the one that we know is least-squares optimal (see Hubert, Arabie, and Meulman, 2002, for an explicit justification of optimality using a dynamic programming routine).

```
>> load number.dat
>> inperm = [1 2 3 4 5 6 7 8 9 10];
>> [fit diff coord] = linfit(number,inperm);
>> coord'
ans =
  Columns 1 through 6
   -0.5345   -0.4050   -0.3258   -0.1988   -0.0842    0.0566
  Columns 7 through 10
    0.1492    0.2608    0.4247    0.6570
>> diff
diff =
    2.1046
>> inperm = [1 2 3 5 4 6 7 9 10 8];
>> [fit diff coord] = linfit(number,inperm);
>> coord'
ans =
  Columns 1 through 6
   -0.6570   -0.4247   -0.2608   -0.1492   -0.0566    0.0842
  Columns 7 through 10
    0.1988    0.3258    0.4050    0.5345
>> diff
diff =
    1.9599
```

1.3.2 The monotonic transformation of a proximity matrix using the MATLAB function proxmon.m

The MATLAB function, `proxmon.m`, provides a monotonically transformed proximity matrix that is close in a least-squares sense to a given input matrix. The syntax is

```
[monproxpermut vaf diff] = proxmon(proxpermut,fitted)
```

Here, `PROXPERMUT` is the input proximity matrix (which may have been subjected to an initial row/column permutation, hence the suffix '`PERMUT`') and `FITTED` is a given target matrix; the output matrix `MONPROXPERMUT` is closest to `FITTED` in a least-squares sense and obeys the order constraints obtained from each pair of entries in (the upper-triangular portion of) `PROXPERMUT` (and where the inequality constrained optimization is carried out using the Dykstra-Kaczmarz iterative projection strategy); `VAF` denotes 'variance-accounted-for' and indicates how much variance in `MONPROXPERMUT` can be accounted for by `FITTED`; finally,`DIFF` is the value of the least-squares loss function and is (one-half) the sum of squared differences between the entries in `FITTED` and `MONPROXPERMUT`.

In the notation of the previous section when fitting a given order, `FITTED` would correspond to the matrix $\{|x_j - x_i|\}$, where $x_1 \leq x_2 \leq \cdots \leq x_n$; the input `PROXPERMUT` would be $\{p_{\rho^0(i)\rho^0(j)}\}$; `MONPROXPERMUT` would be $\{f(p_{\rho^0(i)\rho^0(j)})\}$, where the function $f(\cdot)$ satisfies the monotonicity constraints, i.e., if $p_{\rho^0(i)\rho^0(j)} < p_{\rho^0(i')\rho^0(j')}$ for $1 \leq i < j \leq n$ and $1 \leq i' < j' \leq n$, then $f(p_{\rho^0(i)\rho^0(j)}) \leq f(p_{\rho^0(i')\rho^0(j')})$. The transformed proximity matrix $\{f(p_{\rho^0(i)\rho^0(j)})\}$ minimizes the least-squares criterion (`DIFF`) of

$$\sum_{i<j}(f(p_{\rho^0(i)\rho^0(j)}) - |x_j - x_i|)^2,$$

over all functions $f(\cdot)$ that satisfy the monotonicity constraints. The `VAF` is a normalization of this loss value by the sum of squared deviations of the transformed proximities from their mean:

$$\text{VAF} = 1 - \frac{\sum_{i<j}(f(p_{\rho^0(i)\rho^0(j)}) - |x_j - x_i|)^2}{\sum_{i<j}(f(p_{\rho^0(i)\rho^0(j)}) - \bar{f})^2},$$

where $\bar{f}$ denotes the mean of the off-diagonal entries in $\{f(p_{\rho^0(i)\rho^0(j)})\}$.

An application incorporating proxmon.m

The script m-file listed below gives an application of `proxmon.m` using the (globally optimal) permutation found previously for our `number.dat` matrix. First, `linfit.m` is invoked to obtain a fitted matrix (`fit`); `proxmon.m` then generates the monotonically transformed proximity matrix (`monproxpermut`) with `vaf` = .5821 and `diff` = 1.0623. The strategy is then repeated cyclically (i.e., finding a fitted matrix based on the monotonically transformed proximity matrix, finding a new monotonically transformed matrix, and so on). To avoid degeneracy (where all matrices would converge to zeros), the sum of squares of the fitted matrix is kept the same as it was initially; convergence is based on observing a minimal change (less than 1.0e-006) in the `vaf`. As indicated in the output below, the final `vaf` is .6672 with a `diff` of .9718. (Although the permutation found earlier for `number.dat` remains the same throughout the construction of the optimal monotonic transformation, in this particular example it would also remain optimal with the same vaf if the unidimensional scaling was repeated with `monproxpermut` now considered the input proximity matrix. Even though probably rare, other data sets might not have such an invariance, and it may be desirable to initiate an iterative routine that finds both a unidimensional scaling [i.e., an object ordering] in addition to monotonically transforming the proximity matrix.)

```
load number.dat
inperm = [8 10 9 7 6 4 5 3 2 1];
[fit diff coord] = linfit(number,inperm);
[monproxpermut vaf diff] = ...
    proxmon(number(inperm,inperm),fit);
sumfitsq = sum(sum(fit.^2));
prevvaf = 2;
while (abs(prevvaf-vaf) >= 1.0e-006)
   prevvaf = vaf;
   [fit diff coord] = linfit(monproxpermut,1:10);
   sumnewfitsq = sum(sum(fit.^2));
   fit = sqrt(sumfitsq)*(fit/sqrt(sumnewfitsq));
    [monproxpermut vaf diff] = proxmon(number(inperm,inperm), fit);
end

fit
diff
coord'
monproxpermut
vaf

fit =
  Columns 1 through 6
         0    0.0824    0.1451    0.3257    0.4123    0.5582
    0.0824         0    0.0627    0.2432    0.3298    0.4758
    0.1451    0.0627         0    0.1806    0.2672    0.4131
    0.3257    0.2432    0.1806         0    0.0866    0.2325
    0.4123    0.3298    0.2672    0.0866         0    0.1459
    0.5582    0.4758    0.4131    0.2325    0.1459         0
    0.5834    0.5010    0.4383    0.2578    0.1711    0.0252
    0.7244    0.6419    0.5793    0.3987    0.3121    0.1662
    0.8696    0.7872    0.7245    0.5440    0.4573    0.3114
    1.2231    1.1406    1.0780    0.8974    0.8108    0.6649
  Columns 7 through 10
    0.5834    0.7244    0.8696    1.2231
    0.5010    0.6419    0.7872    1.1406
    0.4383    0.5793    0.7245    1.0780
    0.2578    0.3987    0.5440    0.8974
    0.1711    0.3121    0.4573    0.8108
    0.0252    0.1662    0.3114    0.6649
         0    0.1410    0.2862    0.6397
    0.1410         0    0.1452    0.4987
    0.2862    0.1452         0    0.3535
    0.6397    0.4987    0.3535         0
diff =
    0.9718
ans =
  Columns 1 through 6
   -0.4558   -0.3795   -0.3215   -0.1544   -0.0742    0.0609
  Columns 7 through 10
    0.0842    0.2147    0.3492    0.6764
monproxpermut =
  Columns 1 through 6
         0    0.2612    0.2458    0.2612    0.2458    0.5116
    0.2612         0    0.2458    0.2458    0.4286    0.2458
    0.2458    0.2458         0    0.2458    0.5116    0.6899
    0.2612    0.2458    0.2458         0    0.2458    0.2458
    0.2458    0.4286    0.5116    0.2458         0    0.2612
    0.5116    0.2458    0.6899    0.2458    0.2612         0
    0.6080    0.5116    0.2458    0.2458    0.2458    0.2458
    0.6899    0.7264    0.2458    0.2612    0.5116    0.2458
    0.5116    0.5116    0.6899    0.6080    0.4286    0.2458
    1.2231    1.1406    1.0780    0.6899    0.7264    0.6080
  Columns 7 through 10
    0.6080    0.6899    0.5116    1.2231
    0.5116    0.7264    0.5116    1.1406
    0.2458    0.2458    0.6899    1.0780
    0.2458    0.2612    0.6080    0.6899
    0.2458    0.5116    0.4286    0.7264
    0.2458    0.2458    0.2458    0.6080
         0    0.1410    0.5116    0.6080
    0.1410         0    0.2458    0.4286
    0.5116    0.2458         0    0.2612
    0.6080    0.4286    0.2612         0
vaf =
    0.6672
```

1.4 Appendix: The Dykstra-Kaczmarz Method for Solving Linear (In)equality Constrained Least-Squares Tasks

Kaczmarz's method can be characterized as follows:

Given $\mathbf{A} = \{a_{ij}\}$ of order $m \times n$, $\mathbf{x}' = \{x_1, \ldots, x_n\}$, $\mathbf{b}' = \{b_1, \ldots, b_m\}$, and assuming the linear system $\mathbf{Ax} = \mathbf{b}$ is consistent, define the set $C_i = \{\mathbf{x} \mid a_{ij}x_j = b_i\}$, for $1 \leq i \leq m$. The projection of any $n \times 1$ vector $\mathbf{y}$ onto C_i is simply $\mathbf{y} - (\mathbf{a}_i'\mathbf{y} - b_i)\mathbf{a}_i(\mathbf{a}_i'\mathbf{a}_i)^{-1}$, where $\mathbf{a}_i' = \{a_{i1}, \ldots, a_{in}\}$. Beginning with a vector $\mathbf{x}_0$, and successively projecting $\mathbf{x}_0$ onto C_1, and that result onto C_2, and so on, and cyclically and repeatedly reconsidering projections onto the sets $C_1, \ldots, C_m$, leads at convergence to a vector $\mathbf{x}_0^*$ that is closest to $\mathbf{x}_0$ (in vector 2-norm, so $\sum_{i=1}^{n}(x_{0i} - x_{0i}^*)^2$ is minimized) and $\mathbf{Ax}_0^* = \mathbf{b}$. In short, Kaczmarz's method provides an iterative way to solve least-squares tasks subject to equality restrictions.

Dykstra's method can be characterized as follows:

Given $\mathbf{A} = \{a_{ij}\}$ of order $m \times n$, $\mathbf{x}_0' = \{x_{01}, \ldots, x_{0n}\}$, $\mathbf{b}' = \{b_1, \ldots, b_m\}$, and $\mathbf{w}' = \{w_1, \ldots, w_n\}$, where $w_j > 0$ for all j, find $\mathbf{x}_0^*$ such that $\mathbf{a}_i'\mathbf{x}_0^* \leq b_i$ for $1 \leq i \leq m$ and $\sum_{i=1}^{n} w_i(x_{0i} - x_{0i}^*)^2$ is minimized. Again, (re)define the (closed convex) sets $C_i = \{\mathbf{x} \mid a_{ij}x_j \leq b_i\}$ and when a vector $\mathbf{y} \notin C_i$, its projection onto C_i (in the metric defined by the weight vector $\mathbf{w}$) is $\mathbf{y} - (\mathbf{a}_i'\mathbf{y} - b_i)\mathbf{a}_i\mathbf{W}^{-1}(\mathbf{a}_i'\mathbf{W}^{-1}\mathbf{a}_i)^{-1}$, where $\mathbf{W}^{-1} = \text{diag}\{w_1^{-1}, \ldots, w_n^{-1}\}$. We again initialize the process with the vector $\mathbf{x}_0$ and each set $C_1, \ldots, C_m$ is considered in turn. If the vector being carried forward to this point when C_i is (re)considered does not satisfy the constraint defining C_i, a projection onto C_i occurs. The sets $C_1, \ldots, C_m$ are cyclically and repeatedly considered but with one difference from the operation of Kaczmarz's method — each time a constraint set C_i is revisited, any changes from the previous time C_i was reached are first "added back". This last process ensures convergence to an optimal solution $\mathbf{x}_0^*$ (see Dykstra, 1983). Thus, Dykstra's method generalizes the equality restrictions that can be handled by Kaczmarz's strategy to the use of inequality constraints.

Chapter 2

Linear Multidimensional Scaling

Chapter 1 gave an optimization strategy based on iterative quadratic assignment for the linear unidimensional scaling (LUS) task in the L_2-norm, with all implementations carried out within a MATLAB computational environment. The central LUS task involves arranging the n objects in a set $S = \{O_1, O_2, \ldots, O_n\}$ along a single dimension, defined by coordinates $x_1, x_2, \ldots, x_n$, based on an $n \times n$ symmetric proximity matrix $\mathbf{P} = \{p_{ij}\}$, whose nonnegative entries are given a dissimilarity interpretation ($p_{ij} = p_{ji}$ for $1 \leq i, j \leq n$; $p_{ii} = 0$ for $1 \leq i \leq n$). The L_2 criterion

$$\sum_{i<j}(p_{ij} - |x_j - x_i|)^2, \tag{2.1}$$

is minimized by the choice of the coordinates. The present chapter will give extensions to multidimensional scaling in the city-block metric for the L_2 norm. The computational routines to be discussed and illustrated are again freely available as MATLAB m-files. We also note that most of the references given in Chapter 1 would also be relevant here as background material on the basic LUS task, but that review will not be repeated. Also, we will not discuss (in this chapter) comparisons to other methods (or strategies) for multidimensional scaling in the city-block metric — for the development of some of these alternatives, see Brusco (2001), Brusco and Stahl (in press), Groenen, Heiser, and Meulman (1999), Hubert, Arabie, and Meulman (1997), and Hubert, Arabie, and Hesson-McInnis (1992).

In the extensions to city-block multidimensional scaling being pursued, a slight generalization to the basic unidimensional task that incorporates an additional additive constant will prove extremely convenient. So, in Section 2.1 we emphasize the more general least-squares loss function of the form

$$\sum_{i<j}(p_{ij} - \{|x_j - x_i| - c\})^2, \tag{2.2}$$

where c is some constant to be estimated along with the coordinates $x_1, \ldots, x_n$. Section 2.2 removes the restriction to fitting only a single unidimensional structure to a symmetric proximity matrix, and relies on the type of computational approaches developed in Section 2.1 that include the augmentation by estimated additive constants. Based on these latter strategies, extensions are given to the use of multiple unidimensional structures through a procedure of successive residualization of the original proximity matrix (even though in this process, negative residuals are encountered and need to be fitted). For example, the fitting of two LUS structures to a proximity matrix $\{p_{ij}\}$ could be rephrased as the minimization of an L_2 loss function generalizing (2.2) to the form

$$\sum_{i<j}(p_{ij} - [|x_{j1} - x_{i1}| - c_1] - [|x_{j2} - x_{i2}| - c_2])^2. \tag{2.3}$$

The attempt to minimize (2.3) could proceed with the fitting of a single LUS structure to $\{p_{ij}\}$, $[|x_{j1} - x_{i1}| - c_1]$, and once obtained, fitting a second LUS structure, $[|x_{j2} - x_{i2}| - c_2]$, to the residual matrix, $\{p_{ij} - [|x_{j1} - x_{i1}| - c_1]\}$. The process would then cycle by repetitively fitting the residuals from the second linear structure by the first, and the residuals from the first linear structure by the second, until the sequence converges. In any case, obvious extensions would also exist to (2.3) for the inclusion of more than two LUS structures.

The explicit inclusion of two constants, c_1 and c_2, in (2.3) rather than adding these two together and including a single additive constant c, deserves some additional introductory explanation. As would be the case in fitting a single LUS structure using the loss functions in (2.2), two interpretations exist for the role of the additive constant c. We could consider $\{|x_j - x_i|\}$ to be fitted to the translated proximities $\{p_{ij} + c\}$, or alternatively, $\{|x_j - x_i| - c\}$ to be fitted to the original proximities $\{p_{ij}\}$, where the constant c becomes part of the actual model. Although these two interpretations do not lead to any algorithmic differences in how we would proceed with minimizing the loss functions in (2.2), a consistent use of the second interpretation suggests that we frame extensions to the use of multiple LUS structures as we did in (2.3), where it is explicit that the constants c_1 and c_2 are part of the actual models to be fitted to the (untransformed) proximities $\{p_{ij}\}$. Once c_1 and c_2 are obtained, they could be summed as $c = c_1 + c_2$, and an interpretation made that we have attempted to fit a transformed set of proximities $\{p_{ij} + c\}$ by the sum $\{|x_{j1} - x_{i1}| + |x_{j2} - x_{i2}|\}$ (and in this latter case, a more usual terminology would be one of a two-dimensional scaling (MDS) based on the city-block distance function). However, such a further interpretation is unnecessary and could lead to at least some small terminological confusion in further extensions that we might wish to pursue. For instance, if some type of (optimal nonlinear) transformation, say $f(\cdot)$, of the proximities is also sought (e.g., a monotonic function of some form as we do in Section 2.3) in addition to fitting multiple LUS structures, and where p_{ij} in (2.3) is replaced by $f(p_{ij})$, and $f(\cdot)$ is to be constructed, the first interpretation would require the use of a 'doubly transformed' set of proximities $\{f(p_{ij}) + c\}$ to be fitted by the sum $\{|x_{j1} - x_{i1}| + |x_{j2} - x_{i2}|\}$. In general, it seems best to avoid the need to incorporate the notion of a double transformation in this context, and instead merely consider the constants c_1 and c_2 to be part of the models being fitted to a transformed set of proximities $f(p_{ij})$.

2.1 The Incorporation of Additive Constants in LUS

In Section 2.1.1 below, we present and illustrate a MATLAB m-function, `linfitac.m`, that fits in L_2 a given single unidimensional scale (by providing the coordinates $x_1, \ldots, x_n$) and the additive constant (c) for some fixed input object ordering along the continuum defined by a permutation $\rho^{(0)}$. This parallels directly the m-function given in the previous chapter called `linfit.m`, but now with an included additive constant estimation. The computational mechanisms implemented in `linfitac.m` are reviewed in Section 2.1.1.

2.1.1 The L_2 Fitting of a Single Unidimensional Scale (with an Additive Constant)

Given a fixed object permutation, $\rho^{(0)}$, we denote the set of all $n \times n$ matrices that are additive translations of the off-diagonal entries in the reordered symmetric proximity matrix $\{p_{\rho^{(0)}(i)\rho^{(0)}(j)}\}$ by $\Delta_{\rho^{(0)}}$, and let Ξ be the set of all $n \times n$ matrices that represent the interpoint distances between all pairs of n coordinate locations along a line. Explicitly,

$\Delta_{\rho^{(0)}} \equiv \{\{q_{ij}\}\}$, where $q_{ij} = p_{\rho^{(0)}(i)\rho^{(0)}(j)} + c$, for some constant c, $i \neq j; q_{ii} = 0, 1 \leq i, j \leq n$;

$\Xi \equiv \{\{r_{ij}\}\}$, where $r_{ij} = |x_j - x_i|$ for some set of n coordinates, $x_1 \leq \cdots \leq x_n$; $\sum_i x_i = 0$. Alternatively, we could define Ξ through a set of linear inequality (for non-negativity restrictions) and equality constraints (to represent the additive nature of distances along a line – as we did in `linfit.m` in the previous chapter). In any case, both $\Delta_{\rho^{(0)}}$ and Ξ are closed convex sets (in a Hilbert space), and thus, given any $n \times n$ symmetric matrix with a zero main diagonal, its projection onto either $\Delta_{\rho^{(0)}}$ or Ξ exists, i.e., there is a (unique) member of $\Delta_{\rho^{(0)}}$ or Ξ at a closest (Euclidean) distance to the given matrix (e.g., see Cheney and Goldstein, 1959). Moreover, if a procedure of alternating projections onto $\Delta_{\rho^{(0)}}$ and Ξ is carried out (where a given matrix is first projected onto one of the sets, and that result is then projected onto the second which result is in turn projected back onto the first, and so on), the process is convergent and generates members of $\Delta_{\rho^{(0)}}$ and Ξ that are closest to each other (again, this last statement is justified in Cheney and Goldstein, 1959, Theorems 2 and 4).

Given any $n \times n$ symmetric matrix with a main diagonal of all zeros, which we denote arbitrarily as $\mathbf{U} = \{u_{ij}\}$, its projection onto $\Delta_{\rho^{(0)}}$ may be obtained by a simple formula for the sought constant c. Explicitly, the minimum over c of

$$\sum_{i<j} (\{p_{\rho^{(0)}(i)\rho^{(0)}(j)}\} + c - u_{ij})^2,$$

is obtained for

$$\hat{c} = (2/n(n-1)) \sum_{i<j} (u_{ij} - p_{\rho^{(0)}(i)\rho^{(0)}(j)}),$$

and thus, this last value defines a constant translation of the proximities necessary to generate that member of $\Delta_{\rho^{(0)}}$ closest to $\mathbf{U} = \{u_{ij}\}$. For the second necessary projection and given any $n \times n$ symmetric matrix (again with a main diagonal of all zeros), that we denote arbitrarily as $\mathbf{V} = \{v_{ij}\}$ (but which in our applications will generally have the form $v_{ij} = p_{\rho^{(0)}(i)\rho^{(0)}(j)} + c$ for $i \neq j$ and some constant c), its projection onto Ξ is somewhat more involved and requires minimizing

$$\sum_{i<j}(v_{ij} - r_{ij})^2,$$

over r_{ij}, where $\{r_{ij}\}$ is subject to the linear inequality nonnegativity constraints, and the linear equality constraints of representing distances along a line (of the set Ξ). Although this is a (classic) quadratic programming problem for which a wide variety of optimization techniques has been published, we adopt (as we did in fitting a LUS without an additive constant in `linfit.m`), the Dykstra-Kaczmarz iterative projection strategy reviewed in the addendum (Section 1.4) to Chapter 1.

The MATLAB function linfitac.m

As discussed above, the MATLAB m-function, `linfitac.m`, fits a set of coordinates to a given proximity matrix based on some given input permutation, say, $\rho^{(0)}$, plus an additive constant, c. The usage syntax of

```
[fit vaf coord addcon] = linfitac(prox,inperm)
```

is similar to that of `linfit.m` except for the inclusion (as output) of the additive constant `ADDCON`, and the replacement of the least-squares criterion of `DIFF` by the variance-accounted-for (`VAF`) given by the general formula

$$\text{vaf} = 1 - \frac{\sum_{i<j}(p_{\rho^{(0)}(i)\rho^{(0)}(j)} + c - |x_j - x_i|)^2}{\sum_{i<j}(p_{ij} - \bar{p})^2},$$

where $\bar{p}$ is the mean of the proximity values being used.

To illustrate the invariance of `VAF` to the use of linear transformations of the proximity matrix (although `COORD` and `ADDCON` obviously will change depending on the transformation used), we fit the permutation found optimal to two different matrices: the original proximity matrix for `number.dat`, and one standardized to mean zero and variance one. The latter matrix is obtained with the utility `proxstd.m`, with usage explained in its m-file header comments.

In the recording below (as well as earlier in Chapter 1), semicolons are placed after the invocation of the m-functions to initially suppress the output; transposes(') are then used on the output vectors to conserve space by only using row (as opposed to column) vectors in the listing; also, to conserve space, blank lines are typically deleted in any output given throughout the chapters. Note that for the two proximity matrices used, the vaf values are the same (.5612) but the coordinates and additive constants differ; a listing of the standardized proximity matrix is given in the output to explicitly show how negative proximities pose no problem for the fitting process that allows the incorporation of additive constants within the fitted model.

```
>> load number.dat
>> inperm = [1 2 3 5 4 6 7 9 10 8];
>> [fit vaf coord addcon] = linfitac(number,inperm);
>> vaf
vaf =
    0.5612
>> coord'
ans =
  Columns 1 through 5
   -0.3790   -0.2085   -0.1064   -0.0565   -0.0257
  Columns 6 through 10
    0.0533    0.1061    0.1714    0.1888    0.2565
>> addcon
addcon =
   -0.3089
>> numberstan = proxstd(number,0.0)
numberstan =
  Columns 1 through 5
         0   -0.5919    0.2105    0.8258    0.7027
   -0.5919         0   -1.2663   -0.9611    0.5157
    0.2105   -1.2663         0   -0.9217   -2.3739
    0.8258   -0.9611   -0.9217         0   -0.6313
    0.7027    0.5157   -2.3739   -0.6313         0
    1.2934    0.2302    0.6387   -0.5525   -0.6510
    1.2147    1.0670   -0.5919   -1.1876   -0.7544
    1.8103    0.4369    1.2541    0.2498    0.9882
    1.3771    1.2294   -0.8577    1.2934   -1.4534
    1.5199    0.4123    1.3131   -1.3697    0.6978
  Columns 6 through 10
    1.2934    1.2147    1.8103    1.3771    1.5199
    0.2302    1.0670    0.4369    1.2294    0.4123
    0.6387   -0.5919    1.2541   -0.8577    1.3131
   -0.5525   -1.1876    0.2498    1.2934   -1.3697
   -0.6510   -0.7544    0.9882   -1.4534    0.6978
         0   -0.7150   -0.6953    0.6387    0.2498
   -0.7150         0   -0.6116   -0.9414   -1.2072
   -0.6953   -0.6116         0   -0.6953   -0.4049
    0.6387   -0.9414   -0.6953         0   -0.7347
    0.2498   -1.2072   -0.4049   -0.7347         0
>> [fit vaf coord addcon] = linfitac(numberstan,inperm);
>> vaf
vaf =
    0.5612
>> coord'
```

```
ans =
  Columns 1 through 5
   -1.8656   -1.0262   -0.5235   -0.2783   -0.1266
  Columns 6 through 10
    0.2624    0.5224    0.8435    0.9292    1.2626
>> addcon
addcon =
    1.1437
```

2.2 Finding and Fitting Multiple Unidimensional Scales

As reviewed in the introduction, the fitting of multiple unidimensional structures will be done by (repetitive) successive residualization, along with a reliance on the m-function, `linfitac.m`, to fit each separate unidimensional structure, including its associated additive constant. The m-function for this two-dimensional scaling, `biscalqa.m`, is a bi-dimensional strategy for the L_2 loss function of (2.3). It has the syntax

```
[outpermone outpermtwo coordone coordtwo fitone fittwo ...
addconone addcontwo vaf] = biscalqa(prox,...
targone,targtwo,inpermone,inpermtwo,kblock,nopt)
```

where the variables are similar to `linfitac.m`, but with a suffix of `ONE` or `TWO` to indicate which one of the two unidimensional structures is being referenced. The new variable `NOPT` controls the confirmatory or exploratory fitting of the two unidimensional scales; a value of `NOPT = 0` will fit in a confirmatory manner the two scales indicated by `INPERMONE` and `INPERMTWO`; if `NOPT = 1`, iterative quadratic assignment (QA) is used to locate the better permutations to fit.

In the example given below, the input `PROX` is the standardized (to a mean of zero and a standard deviation of one) 10×10 proximity matrix based on `number.dat` (referred to as `STANNUMBER`); `TARGONE` and `TARGTWO` are identical 10×10 equally-spaced target matrices; `INPERMONE` and `INPERMTWO` are different random permutations of the first 10 integers; `KBLOCK` is set at 2 (for the iterative QA subfunctions). In the output, `OUTPERMONE` and `OUTPERMTWO` refer to the object orders; `COORDONE` and `COORDTWO` give the coordinates; `FITONE` and `FITTWO` are based on the absolute coordinate differences for the two unidimensional structures; `ADDCONONE` and `ADDCONTWO` are the two associated additive constraints; and finally, `VAF` is the variance-accounted-for in `PROX` by the two-dimensional structure.

```
>> load number.dat
>> stannumber = proxstd(number,0.0);
>> inpermone = randperm(10);
>> inpermtwo = randperm(10);
>> kblock = 2;
>> nopt = 1;
>> targone = targlin(10);
>> targtwo = targone;
>> [outpermone outpermtwo coordone coordtwo fitone fittwo...
addconone addcontwo vaf] = biscalqa(stannumber,targone,...
targtwo,inpermone,inpermtwo,kblock,nopt);
>> outpermone
outpermone =
  Columns 1 through 10
     1     2     3     4     5     6     7     9     8    10
>> outpermtwo
outpermtwo =
  Columns 1 through 10
     5     9     3     1     7     4    10     2     8     6
>> coordone'
ans =
  Columns 1 through 5
   -2.1786   -1.2363   -0.5418   -0.2915    0.0009
  Columns 6 through 10
    0.0858    0.6805    1.0310    1.0310    1.4191
>> coordtwo'
ans =
  Columns 1 through 5
   -0.8791   -0.8791   -0.8791   -0.2629   -0.1151
  Columns 6 through 10
    0.2472    0.2472    0.3639    0.9885    1.1688
>> addconone
addconone =
    1.3137
>> addcontwo
addcontwo =
    0.8803
>> vaf
vaf =
    0.8243
```

Although we have used the proximity matrix in `number.dat` primarily as a convenient numerical example to illustrate our various m-functions, the substantive interpretation for this particular two-dimensional structure is rather remarkable and worth pointing out. The first dimension reflects number magnitude perfectly (in its coordinate order) with two objects (the actual digits 7 8) at the same (tied) coordinate value. The second axis reflects the structural characteristics perfectly, with the coordinates split into the odd and even numbers (the digits 4 8 2 0 6 in the first five positions; 3 9 1 7 5 in the second five); there is a grouping of 4 8 2 at the same coordinates (reflecting powers of 2); a grouping of 6 3 9 (reflecting multiples of three) and of 3 9 at the same coordinates (reflecting the powers of 3); the odd numbers 7 5 that are not powers of 3 are at the extreme two coordinates of this second dimension.

Although we will not explicitly illustrate its use here, a tridimensional m-function, `triscalqa.m`, is an obvious generalization of `biscalqa.m`. The pattern of programming that this shows could be used directly as a pattern for extensions beyond three unidimensional structures.

2.3 Incorporating Monotonic Transformation of a Proximity Matrix

As a direct extension of the m-function, `biscalqa.m`, discussed in the last section, the file `bimonscalqa.m`, provides an optimal monotonic transformation (by incorporating the use of `proxmon.m` discussed in Chapter 1) of the original proximity matrix given as input in addition to the later's bidimensional scaling. To prevent degeneracy, the sum-of-squares value for the initial input proximity matrix is maintained in the optimally transformed proximities; the overall strategy is iterative with termination again dependent on a change in the variance-accounted-for being less than 1.0e-005. The usage syntax is almost identical to that of `biscalqa.m` except for the inclusion of the monotonically transformed proximity matrix `MONPROX` as an output matrix:

```
[ ... monprox] = bimonscalqa( ... )
```

The ellipses indicate that the same items should be used as in `biscalqa.m`. If `bimonscalqa` would have been used in the numerical example of the previous section, the same results given would have been provided initially plus the results for the optimally transformed proximity matrix. We give this additional output below, which shows that the incorporation of an optimal monotonic transformation provides an increase in the `VAF` from .8243 to .9362; the orderings on the two dimensions remain the same as well as the nice substantive explanation of the previous section.

```
>> outpermone
outpermone =
     1     2     3     4     5     6     7     9     8    10
>> outpermtwo
outpermtwo =
     9     5     3     1     7     4    10     2     8
>> coordone'
ans =
  Columns 1 through 6
   -2.3514   -1.3290   -0.6409   -0.3565    0.0775    0.1216
  Columns 7 through 10
    0.5857    1.1342    1.1342    1.6247
>> coordtwo'
```

```
ans =
  Columns 1 through 6
   -0.7793   -0.7793   -0.7793   -0.3891   -0.1196    0.3242
  Columns 7 through 10
    0.3242    0.3480    0.8467    1.0035
>> addconone
addconone =
    1.4394
>> addcontwo
addcontwo =
    0.7922
>> vaf
vaf =
    0.9362
>> monprox
monprox =
  Columns 1 through 6
         0   -0.7387   -0.1667    0.5067    0.5067    1.4791
   -0.7387         0   -0.8218   -0.8218    0.5067   -0.1667
   -0.1667   -0.8218         0   -0.8218   -1.6174    0.5067
    0.5067   -0.8218   -0.8218         0   -0.7387   -0.7387
    0.5067    0.5067   -1.6174   -0.7387         0   -0.7387
    1.4791   -0.1667    0.5067   -0.7387   -0.7387         0
    1.0321    0.5067   -0.7387   -0.8218   -0.8218   -0.8218
    2.6590    0.5067    1.0321   -0.1667    0.5067   -0.8218
    1.7609    1.0321   -0.8218    1.0321   -1.2541    0.5067
    2.6231    0.5067    1.4791   -0.8218    0.5067   -0.0534
  Columns 7 through 10
    1.0321    2.6590    1.7609    2.6231
    0.5067    0.5067    1.0321    0.5067
   -0.7387    1.0321   -0.8218    1.4791
   -0.8218   -0.1667    1.0321   -0.8218
   -0.8218    0.5067   -1.2541    0.5067
   -0.8218   -0.8218    0.5067   -0.0534
         0   -0.7387   -0.8218   -0.8218
   -0.7387         0   -0.7387   -0.7387
   -0.8218   -0.7387         0   -0.8218
   -0.8218   -0.7387   -0.8218         0
```

Although we will not provide an example of its use here, trimonscalqa.m, extends triscalqa.m to include an optimal monotonic transformation of whatever is given as the original input proximity matrix.

2.4 Concluding Comments

An obvious conclusion to this chapter is that if one is interested in (nonmetric) city-block scaling in two or three dimensions within L_2, the MATLAB routines referred to in two dimensions as `biscalqa.m` and `bimonscalqa.m`; or in three dimensions as `triscalqa.m` and `trimonscalqa.m`, would be natural alternatives to consider. One aspect of all of these given m-files that we have not emphasized but will in these concluding comments, is their possible usage in the confirmatory context (by setting the `NOPT` switch to `0`), and fitting various fixed object orderings in multiple dimensions. One possible application of this type of confirmatory fitting would be in an individual differences scaling context. Explicitly, we begin with a collection of, say, K proximity matrices, $\mathbf{P}_1, \ldots, \mathbf{P}_K$, obtained from K separate sources, and through some weighting and averaging process construct a single aggregate proximity matrix, $\mathbf{P}_A$. On the basis of $\mathbf{P}_A$, suppose a two-dimensional city-block scaling is constructed (using, say, `biscalqa.m`); we label the latter the "common space" in consistency with what is usually done in the weighted Euclidean model (e.g., see the INDSCAL model of Carroll and Chang, 1970, or the PROXSCAL program in the Categories Module of SPSS — Busing, Commandeur, and Heiser, 1997). Each of the K proximity matrices then can be used in a confirmatory fitting of the object orders along the two axes. Thus, a very general "private space" is generated for each source and where the actual coordinates along both axes are unique to that source, subject only to the object order constraints of the group space. This strategy provides an individual differences model generalization over the usual weighted Euclidean model where the latter allows only differential axes scaling (stretching or shrinking) in generating the private spaces. The authors are continuing to work on these kinds of individual difference generalizations both for multiple unidimensional scalings in L_2 and for other types of proximity matrix representations such as ultrametrics or additive trees.

Chapter 3

Circular Scaling

The major purpose of the present chapter is to discuss circular unidimensional scaling (CUS). Here, the objective is to place the n objects around a closed continuum, such that the reconstructed distance between each pair of objects, defined by the minimum length over the two possible paths that join the objects, reflects the originally given proximities as well as possible. Explicitly, and in analogy with the loss function for linear unidimensional scaling (LUS) in (2.2), we wish to find a set of coordinates, $x_1, \ldots, x_n$, and an $(n+1)^{st}$ value, $x_0 \geq |x_j - x_i|$ for all $1 \leq i \neq j \leq n$, minimizing

$$\sum_{i<j} (p_{ij} + c - \min\{|x_j - x_i|, x_0 - |x_j - x_i|\})^2, \tag{3.1}$$

or equivalently,

$$\sum_{i<j} (p_{ij} - [\min\{|x_j - x_i|, x_0 - |x_j - x_i|\} - c])^2, \tag{3.2}$$

where c is again some constant to be estimated. The value x_0 represents the total length of the closed continuum, and the expression, $\min\{|x_j - x_i|, x_0 - |x_j - x_i|\}$, gives the minimum length over the two possible paths joining objects O_i and O_j. In theory, the CUS task could again be solved by complete enumeration of the loss function in (3.1) over a finite but also typically enormous set for even moderate n. Here, we have all possible distinct object orderings around a closed continuum, $(n-1)!/2$, and for each such ordering, all the possible inflection patterns for where the directionality of the minimum distance calculation changes for the object pairs. Obviously, for general use and analogous to LUS, some type of search strategy is called for to generate the better orderings and inflection patterns around a closed continuum but with feasible computational effort.

The current chapter is organized around the optimization problems posed by CUS and the two main subtasks of obtaining an appropriate object ordering around a closed continuum, and the additional relative placement of the objects according to the directionality of minimum distance calculations. Once these orderings and relative placements have been identified, the estimation of the additive constant in both loss functions (3.1) and (3.2), as well as the identification of the actual coordinates, proceeds through a process of alternating projections onto two closed convex sets. One is defined by the set of all translations of the original proximity values by a constant; the second closed convex set is defined by the collection of all coordinate structures consistent with the given object ordering and the relative object placement that characterizes the directionality of minimum distance calculations around the closed continuum. In the specific contexts we consider, the process of alternating projections is convergent (see Cheney & Goldstein, 1956), and generates a final solution defined by two points within the two convex sets that are closest to each other. Although the emphasis in the present chapter is on a single symmetric proximity matrix defined for one set of objects to be fitted by CUS model, Section 3.2 will also develop a fairly direct extension to the use of sums of such circular structures that can be fitted to a single proximity matrix through successive residualizations of the given matrix (this is analogous to what was done in Chapter 2 for multiple LUS representations).

As a final preliminary note on the data that will be used in this chapter for numerical illustrations, a rather well-known proximity matrix is given in Table 3.1 (and called '`morse_digits.dat`'). The later is a 10×10 proximity matrix for the 10 Morse Code symbols that represent the first ten digits: (0: $- - - - -$; 1: $\bullet - - - -$; 2: $\bullet \bullet - - -$; 3: $\bullet \bullet \bullet - -$; 4: $\bullet \bullet \bullet \bullet -$; 5: $\bullet \bullet \bullet \bullet \bullet$; 6: $- \bullet \bullet \bullet \bullet$; 7: $- - \bullet \bullet \bullet$; 8: $- - - \bullet \bullet$; 9: $- - - - \bullet$). The entries in Table 3.1 have a dissimilarity interpretation and are defined for each object pair by 2.0 minus the sum of the two proportions for a group of subjects used by Rothkopf (1957) representing "same" judgments to the two symbols when given in the two possible presentation orders. Based on previous multidimensional scalings of the complete data set involving all of the Morse code symbols and in which the data of Table 3.1 are embedded (e.g., see Shepard, 1963; Kruskal & Wish, 1978), it might be expected that the symbols for the digits would form a clear linear unidimensional structure that would be interpretable according to a regular progression in the number of dots to dashes. It turns out, as discussed in greater detail below, that a circular model (or actually, a sum of circular structures) is probably more consistent with the patterning of the proximities in Table 3.1 than are representations based on linear unidimensional scalings. (For completeness, we might note that the possible usefulness of a circular model for these specific proximities [but not to the consideration of multiple circular structures] has been pointed out before in the literature, most notably in the two-dimensional metric scaling given as an illustrative example by Mardia, Kent, and Bibby, 1979, p. 404, or in the combinatorial optimization approach of quadratic assignment discussed by Hubert and Schultz, 1976, which is based on permuting the rows and columns of a proximity matrix to achieve a best fit against a fixed target matrix.)

3.1 The Mechanics of CUS

The CUS task as characterized by the loss function in (3.1) can be considered in two stages as with the presentation of LUS. One subtask is the identification of an ordering of the n objects around a closed continuum that again will be denoted by a permutation of the first n integers, $\varphi(\cdot)$, such that $\varphi(i) = j$ if object O_j is placed at position i; here, position 1 is arbitrarily specified at some point along the closed continuum, and the order of the positions

Table 3.1: A proximity matrix, morse_digits.dat, for the 10 Morse code symbols representing the first ten digits (data from Rothkopf, 1957)

0.00	.75	1.69	1.87	1.76	1.77	1.59	1.26	.86	.95
.75	0.00	.82	1.54	1.85	1.72	1.51	1.50	1.45	1.63
1.69	.82	0.00	1.25	1.47	1.33	1.66	1.57	1.83	1.81
1.87	1.54	1.25	0.00	.89	1.32	1.53	1.74	1.85	1.86
1.76	1.85	1.47	.89	0.00	1.41	1.64	1.81	1.90	1.90
1.77	1.72	1.33	1.32	1.41	0.00	.70	1.56	1.84	1.64
1.59	1.51	1.66	1.53	1.64	.70	0.00	.70	1.38	1.70
1.26	1.50	1.57	1.74	1.81	1.56	.70	0.00	.83	1.22
.86	1.45	1.83	1.85	1.90	1.84	1.38	.83	0.00	.41
.95	1.63	1.81	1.86	1.90	1.64	1.70	1.22	.41	0.00

from 1 to n is, for convenience, taken clockwise. In addition to $\varphi(\cdot)$, a set of inflection points must be identified for the n positions to indicate where the minimum distance calculation must change direction around the closed continuum. Explicitly, a set of $n-1$ integers, $1 \leq k_1 \leq \ldots \leq k_{n-1} \leq n$, is sought, where k_i is associated with position i, $1 \leq i \leq n-1$. For positions $i < j$, the minimum distance is in the clockwise direction when $j \leq k_i$, and in the counterclockwise direction when $j > k_i$ (we note that an integer k_n for position n is unnecessary, and any k_i equal to n merely indicates that for all positions j, for $i < j$, the minimum distance is always in the clockwise direction). The second subtask, once given $\varphi(\cdot)$ and $k_1, \ldots, k_{n-1}$, is the estimation of the set of coordinates and the additive constant c to fit the proximities. We again discuss these two subtasks in the reverse order.

3.1.1 The Estimation of c and $\min\{|x_j - x_i|, x_0 - |x_j - x_i|\}$ for a Fixed Permutation and Set of Inflection Points

For notational convenience, the set of all $n \times n$ matrices that are additive translations of the off-diagonal entries in the reordered proximity matrix, $\{p_{\varphi(i)\varphi(j)}\}$, will again be denoted by Δ_φ (see Section 2.1.1); the set of all $n \times n$ matrices that represent the distances around the closed continuum based on the inflection points $k_1, \ldots, k_{n-1}$ will be more fully denoted by $\Xi(k_1, \ldots, k_{n-1})$ and explicitly defined as follows:

$\Xi(k_1, \ldots, k_{n-1}) \equiv \{\{r_{ij}\}\}$, where $r_{ij} = |x_j - x_i|$ for $i < j \leq k_i$; $r_{ij} = x_0 - |x_j - x_i|$ for $i < j, j > k_i$; $r_{ji} = r_{ij}$ for $1 \leq i < j \leq n$; $r_{ii} = 0$ for $1 \leq i \leq n$; for some collection of coordinates, $x_1, \ldots, x_n$, and an $(n+1)^{st}$ value, x_0, where $x_1 \leq \ldots \leq x_n \leq x_0$; $x_1 \equiv 0.0$; and $|x_j - x_i| \leq x_0 - |x_j - x_i|$ for $i < j \leq k_i$; $|x_j - x_i| \geq x_0 - |x_j - x_i|$ for $i < j, j > k_i$.

As noted in this definition, the first position, x_1, is specified without loss of generality to be 0.0; the value, x_0, can either be interpreted as the length of the closed continuum or as a second coordinate value attached to the first position but taken in the clockwise direction. Given Δ_φ and $\Xi(k_1,\ldots,k_{n-1})$ (where the latter can be defined through a set of linear inequality/equality constraints), the process of alternating projections onto Δ_φ and $\Xi(k_1,\ldots,k_{n-1})$ would proceed exactly as in LUS.

3.1.2 Obtaining Object Orderings and Inflection Points Around a Closed Continuum

Identifying an object ordering around a closed continuum to be used in the minimization of the loss function in (3.1) follows exactly the same pattern as for LUS. The cross-product statistic in (1.5) is again maximized but with a different $n \times n$ (target) matrix, $T = \{t_{ij}\}$, initially defined by n positions equally-spaced around a closed continuum, i.e., $t_{ij} = \min\{|i-j|, n-|i-j|\}$ for $1 \le i,j \le n$ (as in LUS, this target could eventually be replaced, now by $t_{ij} = \min\{|x_j - x_i|, x_0 - |x_j - x_i|\}$ based on the outcome of the minimization of (3.1)). Given some best permutation, $\varphi_{K(\cdot)}$, obtained through the initial target and set of local operations on some randomly given initial permutation, a collection of inflection points, $k_1,\ldots,k_{n-1}$, still must be generated before the optimization of (3.1) can continue. This latter task will be approached through a heuristic application of an iterative projection strategy of the same general type developed by Hubert and Arabie (1995) for the fitting of various graph-theoretic structures to a symmetric proximity matrix.

To attempt an identification of $k_1,\ldots,k_{n-1}$ given the permutation $\varphi_{K(\cdot)}$, we begin with the reordered proximity matrix $\{p_{\varphi_{K(i)}\varphi_{K(j)}}\}$, and initialize a process of iterative projection onto the class of constraints given by the structure $\Xi(k_1,\ldots,k_{n-1})$ but with one exception necessitated by the fact that an appropriate set of values for $k_1,\ldots,k_{n-1}$ is not yet known. Explicitly, when considering a pair of positions, $i < j$ $(2 \le j-i)$, and the two possible constraints that could be imposed, i.e., either $r_{i(i+1)} + \cdots + r_{(j-1)j} = r_{ij}$ or $r - (r_{i(i+1)} + \cdots + r_{(j-1)j}) = r_{ij}$ for $r = r_{12} + \cdots + r_{(n-1)n} + r_{1n}$, we select according to which left side is smaller, based on the current entries in the matrix being carried forward to this point, and impose that specific constraint. Otherwise, the process continues cyclically through the whole set of constraints, and for each time a constraint is reconsidered, any changes that were made the previous time the constraint was encountered are first "undone".

Because of the procedure of redressing the (immediately) previous changes each time a constraint is reconsidered, the process just described may not converge and could eventually oscillate through a finite collection of distinct matrices. If such nonconvergence is observed, and previous changes from that point on are not redressed, the process will then converge to a matrix in $\Xi(k_1,\ldots,k_{n-1})$ for some specific values of $k_1,\ldots,k_{n-1}$. A justification for this last assertion of convergence is given by the general results presented in Hubert and Arabie (1995); also, that source provides empirical evidence that as a heuristic optimization strategy, it is generally better to begin with the procedure of redressing previous changes until an oscillation is observed, rather than immediately starting without the process of redressing previous changes (which would also produce a matrix in $\Xi(k_1,\ldots,k_{n-1})$ for some specific $k_1,\ldots,k_{n-1}$). It should also be noted that although convergence to some matrix in $\Xi(k_1,\ldots,k_{n-1})$ is guaranteed by the strategy just described, and thus to an identified fixed collection of inflection points, $k_1, \ldots, k_{n-1}$, the latter matrix may now not be optimal for this collection of inflection points in the minimization of (3.1). Specifically, even though the identification of the collection $k_1, \ldots, k_{n-1}$ can proceed by a process of iterative projection and an updating of a matrix $\{r_{ij}\}$ to produce a member of $\Xi(k_1, \ldots, k_{n-1})$, because of the possible nonconvergence noted above and the subsequent lack of redressing previous changes from that point on, the matrix identified in $\Xi(k_1, \ldots, k_{n-1})$ may not be the best achievable even for this particular collection of inflection points (although in our computational experience it is typically very close to being optimal). Thus, as a "polishing" step to ensure that an optimal member of $\Xi(k_1, \ldots, k_{n-1})$ is identified, the collection $k_1, \ldots, k_{n-1}$ and the permutation $\varphi_K(\cdot)$ should be used anew in the optimization of (3.1) to obtain the optimal target matrix, $\{\min\{|x_j - x_i|, x_0 - |x_j - x_i|\}\}$.

3.1.3 The Circular Unidimensional Scaling Utilities, cirfit.m and cirfitac.m

The two circular unidimensional scaling utilities, `cirfit.m` and `cirfitac.m`, that implement the mechanics of fitting the CUS model (including the identification of inflection points), parallel the LUS utilities of `linfit.m` and `linfitac.m`. The m-file `cirfit.m` does a confirmatory fitting of a given order (assumed to be an object ordering around a closed unidimensional structure) using Dykstra's (Kaczmarz's) iterative projection least-squares method. The usage syntax is

```
 [fit, diff] = cirfit(prox,inperm)
```

where `INPERM` is the given order; `FIT` is an $n \times n$ matrix that is fitted to `PROX(INPERM,INPERM)` with a least-squares value `DIFF`. The syntax for the routine, `cirfitac.m`, is the same except for the inclusion of an additive constant, `ADDCON`, and the use of `VAF` (variance-accounted-for) rather than `DIFF`:

```
[fit,vaf,addcon] = cirfitac(prox,inperm)
```

In brief, then, the type of matrix being fitted to the proximity matrix has the form

$$\{\min(| x_{\rho(j)} - x_{\rho(i)} |,\ x_0 - | x_{\rho(j)} - x_{\rho(i)} |)\ - c\},$$

where c is an estimated additive constant (assumed equal to zero in `cirfit.m`), $x_{\rho(1)} \leq x_{\rho(2)} \leq \cdots \leq x_{\rho(n)} \leq x_0$, and the last coordinate, x_0, is the circumference of the circular structure. We can obtain these latter coordinates from the adjacent spacings in the output matrix `FIT`.

As an example, we applied `cirfit.m` to `morse_digits` with an assumed identity input permutation; the spacings around the circular structure between the placements for objects 1 and 2 is .5337; 2 and 3: .7534; 3 and 4: .6174; 4 and 5: .1840; 5 and 6: .5747; 6 and 7: .5167; 7 and 8: .3920; 8 and 9: .5467; 9 and 10: .1090; and back around between 10 and 1: .5594. For `cirfitac.m` the additive constant was estimated as -.8031 with a variance-accounted-for of .7051; here, the spacings around the circular structure between the placements for objects 1 and 2 is .2928; 2 and 3: .4322; 3 and 4: .2962; 4 and 5: .0234; 5 and 6: .3338; 6 and 7: .2758; 7 and 8: .2314; 8 and 9: .2800; 9 and 10: .0000; and back around between 10 and 1: .2124.

```
>> load morse_digits.dat
>> morse_digits
morse_digits =
  Columns 1 through 6
         0    0.7500    1.6900    1.8700    1.7600    1.7700
    0.7500         0    0.8200    1.5400    1.8500    1.7200
    1.6900    0.8200         0    1.2500    1.4700    1.3300
    1.8700    1.5400    1.2500         0    0.8900    1.3200
    1.7600    1.8500    1.4700    0.8900         0    1.4100
    1.7700    1.7200    1.3300    1.3200    1.4100         0
    1.5900    1.5100    1.6600    1.5300    1.6400    0.7000
    1.2600    1.5000    1.5700    1.7400    1.8100    1.5600
    0.8600    1.4500    1.8300    1.8500    1.9000    1.8400
    0.9500    1.6300    1.8100    1.8600    1.9000    1.6400
  Columns 7 through 10
    1.5900    1.2600    0.8600    0.9500
    1.5100    1.5000    1.4500    1.6300
    1.6600    1.5700    1.8300    1.8100
    1.5300    1.7400    1.8500    1.8600
    1.6400    1.8100    1.9000    1.9000
    0.7000    1.5600    1.8400    1.6400
         0    0.7000    1.3800    1.7000
    0.7000         0    0.8300    1.2200
    1.3800    0.8300         0    0.4100
    1.7000    1.2200    0.4100         0
>> [fit,diff] = cirfit(morse_digits,1:10)
fit =
  Columns 1 through 6
         0    0.5337    1.2871    1.9044    2.0884    2.1237
    0.5337         0    0.7534    1.3707    1.5547    2.1294
    1.2871    0.7534         0    0.6174    0.8014    1.3761
    1.9044    1.3707    0.6174         0    0.1840    0.7587
    2.0884    1.5547    0.8014    0.1840         0    0.5747
    2.1237    2.1294    1.3761    0.7587    0.5747         0
    1.6071    2.1407    1.8927    1.2754    1.0914    0.5167
    1.2151    1.7487    2.2847    1.6674    1.4834    0.9087
    0.6684    1.2021    1.9554    2.2141    2.0301    1.4554
    0.5594    1.0931    1.8464    2.3231    2.1391    1.5644
  Columns 7 through 10
    1.6071    1.2151    0.6684    0.5594
    2.1407    1.7487    1.2021    1.0931
    1.8927    2.2847    1.9554    1.8464
    1.2754    1.6674    2.2141    2.3231
    1.0914    1.4834    2.0301    2.1391
    0.5167    0.9087    1.4554    1.5644
         0    0.3920    0.9387    1.0477
    0.3920         0    0.5467    0.6557
    0.9387    0.5467         0    0.1090
    1.0477    0.6557    0.1090         0
diff =
    7.3898
>> [fit,vaf,addcon] = cirfitac(morse_digits,1:10)
fit =
  Columns 1 through 6
         0    0.2928    0.7250    1.0212    1.0446    0.9996
    0.2928         0    0.4322    0.7284    0.7518    1.0856
    0.7250    0.4322         0    0.2962    0.3196    0.6534
    1.0212    0.7284    0.2962         0    0.0234    0.3572
    1.0446    0.7518    0.3196    0.0234         0    0.3338
    0.9996    1.0856    0.6534    0.3572    0.3338         0
    0.7238    1.0166    0.9292    0.6330    0.6096    0.2758
    0.4924    0.7852    1.1606    0.8644    0.8410    0.5072
    0.2124    0.5052    0.9374    1.1444    1.1210    0.7872
    0.2124    0.5052    0.9374    1.1444    1.1210    0.7872
  Columns 7 through 10
    0.7238    0.4924    0.2124    0.2124
    1.0166    0.7852    0.5052    0.5052
    0.9292    1.1606    0.9374    0.9374
    0.6330    0.8644    1.1444    1.1444
    0.6096    0.8410    1.1210    1.1210
    0.2758    0.5072    0.7872    0.7872
         0    0.2314    0.5114    0.5114
    0.2314         0    0.2800    0.2800
    0.5114    0.2800         0    0.0000
    0.5114    0.2800    0.0000         0
vaf =
    0.7051
addcon =
   -0.8031
```

As a variation on `cirfitac.m`, the m-file `cirfitac_ftarg.m` uses an additional fixed target matrix `TARG` to obtain the inflection points (and therefore, `TARG` should provide a circular ordering). The syntax is otherwise the same as for `cirfitac.m`:

```
[fit,vaf,addcon] = cirfitac_ftarg(prox,inperm,targ)
```

In the example below, an equally-(unit)-spaced circular ordering is used for `TARG` that is obtained from the utility function `targcir.m`; this leads to a (slightly lower compared to `cirfitac.m`) `VAF` of .6670; here, the spacings around the circular structure between the placements for objects 1 and 2 is .3294; 2 and 3: .3204; 3 and 4: .2544; 4 and 5: .0344; 5 and 6: .2837; 6 and 7: .2084; 7 and 8: .3124; 8 and 9: .2701; 9 and 10: .0000; and back around between 10 and 1: .2109.

```
>> load morse_digits.dat
>> targcircular = targcir(10)

targcircular =

     0     1     2     3     4     5     4     3     2     1
     1     0     1     2     3     4     5     4     3     2
     2     1     0     1     2     3     4     5     4     3
     3     2     1     0     1     2     3     4     5     4
     4     3     2     1     0     1     2     3     4     5
     5     4     3     2     1     0     1     2     3     4
     4     5     4     3     2     1     0     1     2     3
     3     4     5     4     3     2     1     0     1     2
     2     3     4     5     4     3     2     1     0     1
     1     2     3     4     5     4     3     2     1     0


>> [fit,vaf,addcon] = cirfitac_ftarg(morse_digits,1:10,targcircular)

fit =

  Columns 1 through 7

         0    0.3294    0.6498    0.9043    0.9387    1.2224    0.7934
    0.3294         0    0.3204    0.5748    0.6093    0.8929    1.1014
    0.6498    0.3204         0    0.2544    0.2888    0.5725    0.7809
    0.9043    0.5748    0.2544         0    0.0344    0.3181    0.5265
    0.9387    0.6093    0.2888    0.0344         0    0.2837    0.4921
    1.2224    0.8929    0.5725    0.3181    0.2837         0    0.2084
    0.7934    1.1014    0.7809    0.5265    0.4921    0.2084         0
    0.4810    0.8104    1.0934    0.8389    0.8045    0.5208    0.3124
    0.2109    0.5403    0.8607    1.1091    1.0747    0.7910    0.5826
    0.2109    0.5403    0.8607    1.1151    1.0747    0.7910    0.5826

  Columns 8 through 10

    0.4810    0.2109    0.2109
    0.8104    0.5403    0.5403
    1.0934    0.8607    0.8607
    0.8389    1.1091    1.1151
    0.8045    1.0747    1.0747
    0.5208    0.7910    0.7910
    0.3124    0.5826    0.5826
         0    0.2701    0.2701
    0.2701         0   -0.0000
    0.2701   -0.0000         0


vaf =

    0.6670


addcon =

   -0.8317
```

The use of a fixed circular target matrix in `cirfitac_ftarg.m` (as opposed to finding one internally as is done in `cirfit.m` and `cirfitac.m`), *could* lead to small anomalies in the results, and the user should be so prepared when using `cirfitac_ftarg.m`. In the example just given, for instance, the (4,10) value (of 1.1151) should probably be 1.1090 to match the (4,9) entry and the fact that 9 and 10 are at tied locations — however, the equally-spaced-circular-target distance from 10 to 4 is shorter clockwise (at a value of 4) than counter-clockwise (at a value of 6), and so the (4,10) value of 1.1151 is taken clockwise (as opposed to 1.1090 if taken counter-clockwise).

The MATLAB function unicirac.m

The MATLAB function m-file, `unicirac.m`, carries out a circular unidimensional scaling of a symmetric dissimilarity matrix (with the estimation of an additive constant) using an iterative quadratic assignment strategy (and thus, is a analogue of `uniscalqa.m` for the LUS task). We begin with an equally-spaced circular target constructed using the m-file `targcir.m` (that could be invoked with the command `targcir(10)`), a (random) starting permutation, and use a sequential combination of the pairwise interchange/rotation/insertion heuristics; the target matrix is re-estimated based on the identified (locally optimal) permutation. The whole process is repeated until no changes can be made in the target or the identified (locally optimal) permutation. The explicit usage syntax is

```
 [fit, vaf, outperm, addcon] = unicirac(prox, inperm, kblock)
```

where the various terms should now be familiar. `INPERM` is a given starting permutation (assumed to be around the circle) of the first n integers; `FIT` is the least-squares optimal matrix (with variance-accounted-for of `VAF`) to `PROX` having the appropriate circular form for the row and column object ordering given by the ending permutation `OUTPERM`. The spacings between the objects are given by the diagonal entries in `FIT` (and the extreme $(1, n)$ entry in `FIT`). `KBLOCK` defines the block size in the use the iterative quadratic assignment routine. The additive constant for the model is given by `ADDCON`.

The problem of local optima are much more severe in circular unidimensional scaling than in LUS. The heuristic identification of inflection points and the relevant spacings can vary slightly depending on the "equivalent" orderings identified around a circular structure. The example given below was identified as the best achievable (and for some multiple number of times) over 100 random starting permutations for `INPERM`; with its vaf of 71.90%, it is apparently the best "attainable". Given the (equivalent to the) identity permutation identified for `outperm`, the substantive interpretation for this representation is fairly clear — we have a nicely interpretable ordering of the Morse code symbols around a circular structure involving a regular replacement of dashes by dots moving clockwise until the symbol containing all dots is reached, and then a subsequent replacement of the dots by dashes until the initial symbol containing all dashes is reached.

```
>> [fit,vaf,outperm,addcon] = ...
unicirac(morse_digits,randperm(10),2)
fit =
  Columns 1 through 6
         0    0.0247    0.3620    0.6413    0.9605    1.1581
    0.0247         0    0.3373    0.6165    0.9358    1.1334
    0.3620    0.3373         0    0.2793    0.5985    0.7961
    0.6413    0.6165    0.2793         0    0.3193    0.5169
    0.9605    0.9358    0.5985    0.3193         0    0.1976
    1.1581    1.1334    0.7961    0.5169    0.1976         0
    1.1581    1.1334    0.7961    0.5169    0.1976    0.0000
    1.0358    1.0606    1.0148    0.7355    0.4163    0.2187
    0.7396    0.7643    1.1016    1.0318    0.7125    0.5149
    0.3883    0.4131    0.7503    1.0296    1.0638    0.8662
  Columns 7 through 10
    1.1581    1.0358    0.7396    0.3883
    1.1334    1.0606    0.7643    0.4131
    0.7961    1.0148    1.1016    0.7503
    0.5169    0.7355    1.0318    1.0296
    0.1976    0.4163    0.7125    1.0638
    0.0000    0.2187    0.5149    0.8662
         0    0.2187    0.5149    0.8662
    0.2187         0    0.2963    0.6475
    0.5149    0.2963         0    0.3513
    0.8662    0.6475    0.3513         0
vaf =
    0.7190
outperm =
     4     5     6     7     8     9    10     1     2     3
addcon =
   -0.7964
```

3.2 Circular Multidimensional Scaling

The discussion in previous sections has been restricted to the fitting of a single circular unidimensional structure to a symmetric proximity matrix. Given the type of computational approach developed for carrying out this task (and, in particular, because of its lack of dependence on the presence of nonnegative proximities), extensions are very direct to the use of multiple unidimensional structures through a process of successive residualization of the original proximity matrix. The fitting of two CUS structures to a proximity matrix generalizes (3.1) to the form

$$\sum_{i<j}(p_{ij}-[\min\{|x_{j1}-x_{i1}|,x_{01}-|x_{j1}-x_{i1}\}-c_1]-[\min\{|x_{j2}-x_{i2}|,x_{02}-|x_{j2}-x_{i2}\}-c_2])^2. \quad (3.3)$$

The attempt to minimize (3.3) could proceed with the fitting of a single CUS structure to $\{p_{ij}\}$, $[\min\{|x_{j1}-x_{i1}|,x_{01}-|x_{j1}-x_{i1}\}-c_1]$, using the computational strategy of Section 3.1, and once obtained, fitting a second CUS structure, $[\min\{|x_{j2}-x_{i2}|,x_{02}-|x_{j2}-x_{i2}|\}-c_2]$ to the residual matrix, $\{p_{ij}-[\min\{|x_{j1}-x_{i1}|,x_{01}-|x_{j1}-x_{i1}|\}]-c_1\}$. The process would then cycle by repetitively fitting the residuals from the second circular structure by the first, and the residuals from the first circular structure by the second, until the sequence converges. In any event, obvious extensions exist for (3.3) to the inclusion of more than two CUS structures or to some mixture of these two, in the spirit of Carroll and Pruzansky's (1980) hybrid models.

The m-function, `bicirac.m`, is a two-(or bi-)dimensional scaling strategy for the L_2 loss function of (3.3), and relies heavily on the m-function `unicirac.m` to fit each separate circular structure, including its associated additive constant. The syntax is

```
[find,vaf,targone,targtwo,outpermone,outpermtwo, addconone, ...
addcontwo] =  bicirac(prox,inperm,kblock)
```

where most of the terms should be familiar from previous usage in, say, `biscalqa.m`. Again, `PROX` is the input proximity matrix ($n \times n$ with a zero main diagonal and a dissimilarity interpretation); `INPERM` is a given starting permutation of the first n integers; `FIND` is the least-squares optimal matrix (with variance-accounted-for of `VAF`) to `PROX` and is the sum of the two circular (anti-Robinson) matrices `TARGONE` and `TARGTWO` based on the two row and column object orderings given by the ending permutations `OUTPERMONE` and `OUTPERMTWO`. `KBLOCK` defines the block size in the use of the iterative quadratic assignment routine and `ADDCONONE` and `ADDCONTWO` are the two additive constants for the two model components.

As an illustration of the results obtainable from the process just described using the Morse code data, the MATLAB output below gives the best (according to a VAF of 92.18%) two-CUS representation obtained from 100 random starting permutations for each of the circular components. The two CUS structures have rather clear substantive interpretations: as with our example using `unicirac.m`, the first shows the regular replacement of dots by dashes moving around the closed continuum; the second provides a perfect ordering around the closed continuum according to ratios of dots to dashes or of dashes to dots and where adjacent pairs of stimuli have dashes and dots exchanged one-for-one, i.e., for the adjacent stimuli pairs moving clockwise, we have: 0:5 for {− − − − −; ● ● ● ● ●●} (0,5); 1:4 for {● − − − −; − ● ● ● ●} (1,6); 2:3 for {● ● − − −; − − ● ● ●} (2,7); 3:2 for {● ● ● − −; − − − ● ●} (3,8); and 1:4 for {− − − − ●; ● ● ● ● −}(4,9). The two additive constants c_1 and c_2 in (3.3) have values of -.7002 and .3521, respectively. (As mentioned, the output given below represents the best two-CUS structures obtained for 100 random starting permutations, but as might be expected given the earlier computational results, the same type of local optima were observed here as found in the fitting of a single CUS structure, i.e., several local optima were generated from small differences in the estimation of inflection points but with the identical object orderings around the closed continua).

```
>> [find,vaf,targone,targtwo,outpermone,outpermtwo,addconone, ...
addcontwo] =  bicirac(morse_digits,randperm(10),2)
find =
  Columns 1 through 6
         0    0.9765    1.4869    1.9626    1.7586    1.7461
    0.9765         0    0.8585    1.5836    1.7815    1.7340
    1.4869    0.8585         0    1.0732    1.4824    1.4414
    1.9626    1.5836    1.0732         0    0.7573    1.3885
    1.7586    1.7815    1.4824    0.7573         0    1.2468
    1.7461    1.7340    1.4414    1.3885    1.2468         0
    1.5637    1.5408    1.6238    1.5709    1.6832    0.7846
    1.4012    1.3783    1.6709    1.7334    1.9374    1.3120
    0.9767    1.4861    1.7787    1.8316    1.8296    1.8771
    0.8569    1.4853    1.8352    1.8882    1.7731    1.8206
  Columns 7 through 10
    1.5637    1.4012    0.9767    0.8569
    1.5408    1.3783    1.4861    1.4853
    1.6238    1.6709    1.7787    1.8352
    1.5709    1.7334    1.8316    1.8882
    1.6832    1.9374    1.8296    1.7731
    0.7846    1.3120    1.8771    1.8206
         0    0.8755    1.4561    1.5759
    0.8755         0    0.9287    1.0485
    1.4561    0.9287         0    0.4679
    1.5759    1.0485    0.4679         0
vaf =
    0.9218
targone =
  Columns 1 through 6
         0    0.2364    0.2680    0.4852    0.7880    1.1894
    0.2364         0    0.0316    0.2488    0.5516    0.9530
    0.2680    0.0316         0    0.2172    0.5199    0.9214
    0.4852    0.2488    0.2172         0    0.3028    0.7042
    0.7880    0.5516    0.5199    0.3028         0    0.4015
    1.1894    0.9530    0.9214    0.7042    0.4015         0
    1.1826    1.3420    1.3104    1.0933    0.7905    0.3890
    1.0800    1.3164    1.3480    1.1958    0.8931    0.4916
    0.6544    0.8908    0.9224    1.1396    1.3187    0.9172
    0.3450    0.5814    0.6130    0.8302    1.1329    1.2266
  Columns 7 through 10
    1.1826    1.0800    0.6544    0.3450
    1.3420    1.3164    0.8908    0.5814
    1.3104    1.3480    0.9224    0.6130
    1.0933    1.1958    1.1396    0.8302
    0.7905    0.8931    1.3187    1.1329
    0.3890    0.4916    0.9172    1.2266
         0    0.1026    0.5282    0.8376
    0.1026         0    0.4256    0.7350
    0.5282    0.4256         0    0.3094
    0.8376    0.7350    0.3094         0
targtwo =
  Columns 1 through 6
         0    0.0491    0.1825    0.3852    0.5267    0.6148
    0.0491         0    0.1334    0.3361    0.4776    0.5657
    0.1825    0.1334         0    0.2027    0.3442    0.4324
    0.3852    0.3361    0.2027         0    0.1415    0.2296
    0.5267    0.4776    0.3442    0.1415         0    0.0882
    0.6148    0.5657    0.4324    0.2296    0.0882         0
    0.6001    0.6427    0.5094    0.3066    0.1652    0.0770
    0.3855    0.4346    0.5679    0.5212    0.3798    0.2916
    0.1270    0.1761    0.3095    0.5122    0.6382    0.5500
    0.0598    0.1089    0.2423    0.4450    0.5865    0.6173
  Columns 7 through 10
    0.6001    0.3855    0.1270    0.0598
    0.6427    0.4346    0.1761    0.1089
    0.5094    0.5679    0.3095    0.2423
    0.3066    0.5212    0.5122    0.4450
    0.1652    0.3798    0.6382    0.5865
    0.0770    0.2916    0.5500    0.6173
         0    0.2146    0.4731    0.5403
    0.2146         0    0.2585    0.3257
    0.4731    0.2585         0    0.0672
    0.5403    0.3257    0.0672         0
outpermone =
     8     9    10     1     2     3     4     5     6     7
outpermtwo =
     7     3     8     4     9    10     5     1     6     2
addconone =
   -0.7002
addcontwo =
    0.3521
```

Chapter 4

LUS for Two-Mode Proximity Data

The proximity data considered thus far for obtaining some type of structural representation have been assumed to be on one intact set of objects, $S = \{O_1, \ldots, O_n\}$, and complete in the sense that proximity values are present between all object pairs. Suppose now that the available proximity data are two-mode, that is *between* two distinct object sets, $S_A = \{O_{1A}, \ldots, O_{n_a A}\}$ and $S_B = \{O_{1B}, \ldots, O_{n_b B}\}$, containing n_a and n_b objects, respectively, and defined through an $n_a \times n_b$ proximity matrix $\mathbf{Q} = \{q_{rs}\}$, where again, for convenience, we assume that the entries in $\mathbf{Q}$ are keyed as dissimilarities. What may be desirable is a joint structural representation of the set $S_A \cup S_B$ (considered as a single object set S containing $n_a + n_b = n$ objects), but one that is based only on the available proximities between the sets S_A and S_B.

A two-mode (dissimilarity matrix) data set for illustrative purposes

To provide a specific example that will be used throughout this chapter as an illustration, Table 4.1 presents an 11×9 two-mode proximity matrix $\mathbf{Q}$ on the absorption of light at 9 different wavelengths by 11 different cones (receptors) in goldfish retina (but in a row and column reordered form that will reflect the discussion to follow). These data are from Schiffman and Falkenberg (1968) (and reanalyzed by Schiffman, Reynolds, and Young, 1981, pp. 328–329), and were originally based on an unpublished doctoral dissertation by Marks (1965). The proximities in the table are (200 minus) the heights of ordinates for particular spectral frequencies as labeled by the columns, and thus, can be considered dissimilarities reflecting the closeness of a particular receptor to a particular wavelength. In terms of the original labeling of the rows as given in Schiffman and Falkenberg, the row permutation in Table 4.1 is (3,8,9,2,6,4,1,7,5,11,10); the column permutation is (4,9,6,5,1,7,2,8,3). The latter column permutation in its given order corresponds to wavelengths of (458):blue-indigo, (430):violet, (485):blue, (498):blue-green, (530):green, (540):green, (585):yellow, (610):orange, (660):red.

Table 4.1: The goldfish_receptor.dat data file constructed from Schiffman and Falkenberg (1968)

47	53	111	143	188	196	200	200	200
48	55	75	100	186	200	200	200	200
46	47	90	125	168	176	177	183	200
99	101	78	60	46	67	107	156	200
122	127	115	79	49	46	91	143	200
115	154	97	73	48	152	84	125	174
198	186	154	148	103	94	63	108	155
135	156	123	127	116	98	49	46	80
141	113	142	148	114	121	61	47	54
173	140	177	176	144	128	64	56	89
200	200	160	161	145	138	80	53	68

4.1 Reordering Two-Mode Proximity Matrices

Given a $n_a \times n_b$ two-mode proximity matrix, $\mathbf{Q}$, defined between the two distinct sets S_A and S_B, it may be desirable at times to have some means for separately reordering the rows and columns of $\mathbf{Q}$ to display some type of pattern that may be present in its entries, or to obtain some joint permutation of the n $(= n_a + n_b)$ row and column objects to effect some further type of simplified representation. These kinds of reordering tasks will be approached with a variant of the quadratic assignment heuristics of the LUS discussion in Chapter 1 applied to a square, $(n_a + n_b) \times (n_a + n_b)$, proximity matrix, $\mathbf{P}^{(tm)}$, in which a two-mode matrix $\mathbf{Q}_{(dev)}$ and its transpose (where $\mathbf{Q}_{(dev)}$ is constructed from $\mathbf{Q}$ by deviating its entries from the mean proximity), form the upper-right- and lower-left-hand portions, respectively, with zeros placed elsewhere. (This use of zero in the presence of deviated proximities, appears a reasonable choice generally in identifying good reorderings of $\mathbf{P}^{(tm)}$. Without this type of deviation strategy, there would typically be no "mixing" of the row and column objects in the permutations that we would identify for the combined (row and column) object set.) Thus, for $\mathbf{0}$ denoting (an appropriately dimensioned) matrix of all zeros,

$$\mathbf{P}^{(tm)} = \begin{bmatrix} \mathbf{0}_{n_a \times n_a} & \mathbf{Q}_{(dev)n_a \times n_b} \\ \mathbf{Q}'_{(dev)n_b \times n_a} & \mathbf{0}_{n_b \times n_b} \end{bmatrix},$$

is the (square) $n \times n$ proximity matrix subjected to a simultaneous row and column reordering, which in turn will induce separate row and column reorderings for the original two-mode proximity matrix $\mathbf{Q}$.

The m-file, `ordertm.m`, implements a quadratic assignment reordering heuristic on the derived matrix $\mathbf{P}^{(tm)}$, with usage

```
[outperm,rawindex,allperms,index,squareprox] = ...
ordertm(proxtm,targ,inperm,kblock)
```

where the two-mode proximity matrix `PROXTM` (with its entries to be deviated from the mean proximity within the use of the m-file) forms the upper-right- and lower-left-hand portions of a defined square ($n \times n$) proximity matrix (`SQUAREPROX`) with a dissimilarity interpretation, and with zeros placed elsewhere (n = number of rows + number of columns of `PROXTM` $= n_a + n_b$); three separate local operations are used to permute the rows and columns of the square proximity matrix to maximize the cross-product index with respect to a square target matrix `TARG`: pairwise interchanges of objects in the permutation defining the row and column order of the square proximity matrix; the insertion of from 1 to `KBLOCK` (which is less than or equal to $n - 1$) consecutive objects in the permutation defining the row and column order of the data matrix; the rotation of from 2 to `KBLOCK` (which is less than or equal to $n - 1$) consecutive objects in the permutation defining the row and column order of the data matrix. `INPERM` is the beginning input permutation (a permutation of the first n integers); `PROXTM` is the two-mode $n_a \times n_b$ input proximity matrix; `TARG` is the $n \times n$ input target matrix. `OUTPERM` is the final permutation of `SQUAREPROX` with the cross-product index `RAWINDEX` with respect to `TARG`. `ALLPERMS` is a cell array containing `INDEX` entries corresponding to all the permutations identified in the optimization from `ALLPERMS{1} = INPERM` to `ALLPERMS{INDEX} = OUTPERM`.

In the example to follow, `ordertm.m`, is used on the dissimilarity matrix of Table 4.1. The square equally-spaced target matrix is obtained from the LUS utility, `targlin.m`. If the listing would be given of the (reordered) matrix, `squareprox(outperm,outperm)`, it would show clearly the unidimensional pattern for a two-mode data matrix that will be explicitly fitted in the next section of this chapter.

```
>> load goldfish_receptor.dat
>> [outperm,rawindex,allperms,index,squareprox] = ...
ordertm(goldfish_receptor,targlin(20),randperm(20),2);
>> outperm
outperm =
  Columns 1 through 11
     1     2    12     3    13    14    15     4     6     5    16
  Columns 12 through 20
    17     7     8    18     9    19    10    11    20
```

4.2 Fitting a Two-Mode Unidimensional Scale

It is possible to fit through iterative projection, best-fitting (in the L_2-norm) unidimensional scales to two-mode proximity data based on a given permutation of the combined row and column object set. Specifically, if $\rho(\cdot)$ denotes some given permutation of the first n integers (where the first n_a integers denote row objects labeled $1, 2, \ldots, n_a$, and the remaining n_b integers denote column objects, labeled $n_a + 1, n_a + 2, \ldots, n_a + n_b (= n)$), we seek a set of coordinates, $x_1 \leq x_2 \leq \cdots \leq x_n$, such that using the reordered square proximity matrix,

$\mathbf{P}_{\rho_0}^{(tm)} = \{p_{\rho_0(i)\rho_0(j)}^{(tm)}\}$, the least-squares criterion

$$\sum_{i,j=1}^{n} w_{\rho_0(i)\rho_0(j)}(p_{\rho_0(i)\rho_0(j)}^{(tm)} - |x_j - x_i|)^2,$$

is minimized, where $w_{\rho_0(i)\rho_0(j)} = 0$ if $\rho_0(i)$ and $\rho_0(j)$ are both row or both column objects, and $= 1$ otherwise. The entries in the matrix fitted to $\mathbf{P}_{\rho_0}^{(tm)}$ are based on the absolute coordinate differences (and which correspond to nonzero values of the weight function $w_{\rho_0(i)\rho_0(j)}$), and thus satisfy certain linear (in)equality constraints generated from how the row and column objects are intermixed by the given permutation $\rho_0(\cdot)$. To give a schematic representation of how these constraints are generated, suppose r_1 and r_2 (c_1 and c_2) denote two arbitrary row (column) objects, and suppose the following 2×2 matrix represents what is to be fit to the four proximity values present between r_1, r_2 and c_1, c_2:

	c_1	c_2
r_1	a	b
r_2	c	d

Depending on how these four objects are ordered (and intermixed) by the permutation $\rho_0(\cdot)$, certain constraints must be satisfied by the entries a, b, c, and d. The representative constraints are given schematically below in terms of the types of intermixing that might be present:

(a) $r_1 \prec r_2 \prec c_1 \prec c_2$ implies $a + d = b + c$;
(b) $r_1 \prec c_1 \prec r_2 \prec c_2$ implies $a + c + d = b$;
(c) $r_1 \prec c_1 \prec c_2 \prec r_2$ implies $a + c = b + d$;
(d) $r_1 \prec r_2 \prec c_1$ implies $c \leq a$;
(e) $r_1 \prec c_1 \prec c_2$ implies $a \leq b$.

The confirmatory unidimensional scaling of a two-mode proximity matrix (based on iterative projection using a given permutation of the row and column objects) is carried out with the m-file, `linfittm`, with usage

```
[fit,diff,rowperm,colperm,coord] = linfittm(proxtm,inperm)
```

here, `PROXTM` is the two-mode proximity matrix, and `INPERM` is the given ordering of the row and column objects pooled together; `FIT` is a $n_a \times n_b$ matrix of absolute coordinate differences fitted to `PROXTM(ROWPERM,COLPERM)`, with `DIFF` being the (least-squares criterion) sum of squared discrepancies between `FIT` and `PROXTM(ROWPERM,COLMEAN)`; `ROWPERM` and `COLPERM` are the row and column object orderings derived from `INPERM`. The $(n_a + n_b) = n$ coordinates (ordered with the smallest such coordinate set at a value of zero) are given in `COORD`.

The example given below uses a permutation obtained from `ordertm.m` on the data matrix `goldfish_receptor.dat`.

```
>> load goldfish_receptor.dat
>> [outperm, rawindex, allperms, index, squareprox] = ...
   ordertm(goldfish_receptor, targlin(20), randperm(20), 2);
>> outperm
outperm =
  Columns 1 through 11
    20    11    10    19     9    18     8     7    17    16     5
  Columns 12 through 20
     6     4    15    14    13     3    12     2     1
>> [fit,diff,rowperm,colperm,coord] = ...
linfittm(goldfish_receptor,outperm);
>> fit
fit =
  Columns 1 through 6
   26.6628   20.7009   50.7896   97.1554  114.8827  175.5191
   37.7739    9.5898   39.6785   86.0443  103.7716  164.4080
   63.3294   15.9658   14.1230   60.4888   78.2160  138.8524
   81.2210   33.8573    3.7686   42.5972   60.3245  120.9609
   83.5516   36.1880    6.0993   40.2665   57.9938  118.6302
  154.9961  107.6324   77.5437   31.1779   13.4506   47.1857
  161.4405  114.0769   83.9882   37.6223   19.8951   40.7413
  171.8850  124.5213   94.4326   48.0668   30.3395   30.2968
  259.1476  211.7840  181.6952  135.3294  117.6022   56.9658
  285.8850  238.5213  208.4326  162.0668  144.3395   83.7032
  294.1072  246.7436  216.6548  170.2890  152.5617   91.9254
  Columns 7 through 9
  190.6100  213.5191  232.4860
  179.4989  202.4080  221.3749
  153.9433  176.8524  195.8193
  136.0518  158.9609  177.9278
  133.7211  156.6302  175.5971
   62.2766   85.1857  104.1527
   55.8322   78.7413   97.7082
   45.3878   68.2968   87.2638
   41.8749   18.9658    0.0011
   68.6122   45.7032   26.7362
   76.8345   53.9254   34.9584
>> diff
diff =
  1.5850e+005
>> rowperm'
ans =
    11    10     9     8     7     5     6     4     3     2     1
```

```
>> colperm'
ans =
     9     8     7     6     5     4     3     2     1
>> coord'
ans =
  Columns 1 through 6
        0   26.6628   37.7739   47.3636   63.3294   77.4524
  Columns 7 through 12
   81.2210   83.5516  123.8182  141.5455  154.9961  161.4405
  Columns 13 through 18
  171.8850  202.1818  217.2727  240.1818  259.1476  259.1487
  Columns 19 through 20
  285.8850  294.1072
```

In complete analogy to what was done in the LUS discussion (with the m-file `linfitac.m` generalizing `linfit.m` by fitting an additive constant along with the absolute coordinate differences), the more general unidimensional scaling model can be fit with an additive constant using the m-file, `linfittmac.m`. Specifically, we now seek a set of coordinates, $x_1 \leq x_2 \leq \cdots \leq x_n$, and an additive constant c, such that using the reordered square proximity matrix, $\mathbf{P}_{\rho_0}^{(tm)} = \{p_{\rho_0(i)\rho_0(j)}^{(tm)}\}$, the least-squares criterion

$$\sum_{i,j=1}^{n} w_{\rho_0(i)\rho_0(j)}(p_{\rho_0(i)\rho_0(j)}^{(tm)} + c - |x_j - x_i|)^2,$$

is minimized, where again $w_{\rho_0(i)\rho_0(j)} = 0$ if $\rho_0(i)$ and $\rho_0(j)$ are both row or both column objects, and $= 1$ otherwise. The m-file usage is

```
[fit,vaf,rowperm,colperm,addcon,coord] = ...
linfittmac(proxtm,inperm)
```

and does a confirmatory two-mode fitting of a given unidimensional ordering of the row and column objects of a two-mode proximity matrix `PROXTM` using Dykstra's (Kaczmarz's) iterative projection least-squares method. It differs from `linfittm.m` by including the estimation of an additive constant, and thus allowing the variance-accounted-for (`VAF`) to be legitimately given as the goodness-of-fit index (as opposed to just `DIFF` as we did in `linfittm.m`). Again, `INPERM` is the given ordering of the row and column objects together; `FIT` is an n_a (number of rows) by n_b (number of columns) matrix of absolute coordinate differences fitted to `PROXTM(ROWPERM,COLPERM)`; `ROWPERM` and `COLPERM` are the row and column object orderings derived from `INPERM`. The estimated additive constant `ADDCON` can be interpreted as being added to `PROXTM` (or alternatively subtracted from the fitted matrix `FIT`).

The same exemplar permutation is used below (as was for `linfittm.m`); following the MATLAB output that now includes the additive constant of -57.7569 and the variance-accounted-for value of .7830, the two unidimensional scalings (in their coordinate forms) are provided in tabular form with an explicit indication of what is a row object (R) and what is a column object (C).

```
>> [fit,vaf,rowperm,colperm,addcon,coord] = ...
linfittmac(goldfish_receptor,outperm);
>> fit
fit =
  Columns 1 through 6
   15.1217   11.7057   29.3422   56.1902   73.9175  103.0501
   25.6629    1.1646   18.8010   45.6491   63.3763   92.5090
   38.9535   12.1261    5.5104   32.3584   50.0857   79.2183
   45.4631   18.6357    0.9993   25.8488   43.5761   72.7087
   46.7026   19.8752    2.2388   24.6093   42.3366   71.4692
   92.1156   65.2881   47.6517   20.8037    3.0764   26.0562
   98.5600   71.7326   54.0962   27.2481    9.5208   19.6118
  109.0045   82.1770   64.5406   37.6926   19.9653    9.1673
  161.5381  134.7107  117.0743   90.2262   72.4989   43.3663
  171.6650  144.8376  127.2012  100.3531   82.6258   53.4932
  179.8873  153.0598  135.4234  108.5753   90.8481   61.7154
  Columns 7 through 9
  118.1410  141.0501  146.4267
  107.5999  130.5090  135.8855
   94.3092  117.2183  122.5949
   87.7996  110.7087  116.0853
   86.5601  109.4692  114.8458
   41.1471   64.0562   69.4328
   34.7027   57.6118   62.9884
   24.2582   47.1673   52.5439
   28.2754    5.3663    0.0103
   38.4023   15.4932   10.1166
   46.6245   23.7154   18.3389
>> vaf
vaf =
    0.7830
>> rowperm'
ans =
    11    10     9     8     7     5     6     4     3     2     1
>> colperm'
ans =
     9     8     7     6     5     4     3     2     1
>> addcon
addcon =
  -57.7569
>> coord'
ans =
```

Table 4.2: The two unidimensional scalings of the goldfish_receptor data

color	number	R or C	no constant	with constant
red (660)	20	C	0.0	0.0
	11	R	26.6628	15.1217
	10	R	37.7739	25.6629
orange (610)	19	C	47.3636	26.8275
	9	R	63.3294	38.9535
yellow (585)	18	C	77.4524	44.4639
	8	R	81.2210	45.4631
	7	R	83.5516	46.7026
green (540)	17	C	123.8182	71.3119
green (530)	16	C	141.5455	89.0392
	5	R	154.9961	92.1156
	6	R	161.4405	98.5600
	4	R	171.8850	109.0045
blue-green (490)	15	C	202.1818	118.1718
blue (485)	14	C	217.2727	133.2627
violet (430)	13	C	240.1818	156.1718
	3	R	259.1476	161.5381
blue-indigo (458)	12	C	259.1487	161.5484
	2	R	285.8850	171.6650
	1	R	294.1072	179.8873

```
Columns 1 through 6
       0   15.1217   25.6629   26.8275   38.9535   44.4639
Columns 7 through 12
 45.4631   46.7026   71.3119   89.0392   92.1156   98.5600
Columns 13 through 18
109.0045  118.1718  133.2627  156.1718  161.5381  161.5484
Columns 19 through 20
171.6650  179.8873
```

4.3 Multiple LUS Reorderings and Fittings

Two m-files are provided that put together the (quadratic assignment) reordering of a two-mode rectangular proximity matrix with the fitting of the unidimensional scale(s). The first, `uniscaltmac.m`, combines the use of `ordertm.m` and `linfittmac.m` along with (re)estimations of the (originally equally-spaced) target matrix using the coordinates obtained until the identified permutation stabilizes. The usage includes the same terms as for the encompassing m-files:

```
[fit, vaf, outperm, rowperm, colperm, addcon, coord] = ...
uniscaltmac(proxtm, inperm, kblock)
```

The second m-file, `biscaltmac.m`, finds and fits, through successive residualization, the sum of two linear unidimensional scales using iterative projection to a two-mode proximity matrix in the L_2-norm based on permutations identified through the use of iterative quadratic assignment. The usage has the form

```
[find,vaf,targone,targtwo,outpermone,outpermtwo, ...
        rowpermone,colpermone,rowpermtwo,colpermtwo,addconone,...
        addcontwo,coordone,coordtwo,axes] = ...
biscaltmac(proxtm,inpermone,inpermtwo,kblock)
```

Most of the terms should be obvious from earlier usage statements; the $n \times 2$ matrix, `AXES`, gives the two-dimensional plotting coordinates for the combined row and column object set.

```
>> [find,vaf,targone,targtwo,outpermone,outpermtwo, ...
        rowpermone,colpermone,rowpermtwo,colpermtwo,addconone,...
        addcontwo,coordone,coordtwo,axes] =...
        biscaltmac(goldfish_receptor,randperm(20),randperm(20),2);
>> find
find =
  Columns 1 through 6
   63.1229   60.0280   94.8707  125.5213  180.1344  208.1426
   54.8267   51.7317   86.5744  117.2251  171.8381  199.8464
   50.9684   45.7140   80.5567  111.2074  165.8204  193.8287
  111.2698  114.3647   79.5220   48.8736   58.9543   86.9626
  137.2291  140.3240  105.4813   74.8307   36.6481   61.0033
  111.4359  114.5309   79.6882   72.2434   58.7882   86.7964
  195.3935  198.4885  163.6458  132.9951   86.6358   75.5565
  143.0070  146.1020  133.4013  139.7799  119.3372  108.2579
  147.5589  130.4909  146.5900  152.9685  132.5259  121.4466
  162.5104  141.9861  161.5415  167.9200  147.4774  136.3981
  194.6519  197.7468  162.9043  169.2829  148.8402  137.7609
  Columns 7 through 9
  200.1002  199.1866  207.6376
  191.8039  190.8903  199.2632
  185.7862  184.8726  193.2455
  101.7749  151.7064  192.9564
   93.5577  143.4893  184.7392
   78.7540  128.3365  169.5865
   58.4163   93.5015  134.7515
   47.1829   60.8001  102.0501
   62.7940   61.8804   88.8614
   70.4843   54.5920   73.9099
   71.8471   58.5882   72.5470
>> vaf
vaf =
    0.9328
>> targone
targone =
  Columns 1 through 6
   17.1701   25.8848   33.5284   45.6645   83.1923  102.7361
    0.2115    8.9261   16.5698   28.7058   66.2337   85.7775
    1.0797    7.6349   15.2786   27.4146   64.9425   84.4863
   50.7605   42.0458   34.4022   22.2661   15.2617   34.8055
   62.5285   53.8138   46.1702   34.0341    3.4937   23.0375
   67.8487   59.1341   51.4904   39.3544    1.8265   17.7173
  110.8711  102.1564   94.5127   82.3767   44.8488   25.3051
  112.0823  103.3676   95.7240   83.5879   46.0600   26.5163
  121.9248  113.2101  105.5665   93.4304   55.9026   36.3588
  121.9910  113.2763  105.6327   93.4966   55.9688   36.4250
  152.6562  143.9415  136.2979  124.1618   86.6340   67.0902
  Columns 7 through 9
  131.6718  156.1808  180.9922
  114.7131  139.2221  164.0335
  113.4220  137.9309  162.7423
   63.7412   88.2502  113.0616
   51.9732   76.4821  101.2936
   46.6530   71.1619   95.9733
    3.6306   28.1396   52.9510
    2.4194   26.9284   51.7398
    7.4231   17.0858   41.8973
    7.4893   17.0196   41.8311
   38.1545   13.6456   11.1659
>> targtwo
targtwo =
  Columns 1 through 6
    8.6234   16.1993   25.0619   28.0089   43.3983   50.4845
    3.8968   11.4727   20.3354   23.2823   38.6718   45.7579
    0.0390    7.5368   16.3995   19.3465   34.7359   41.8221
    5.4725    2.1034   10.9661   13.9130   29.3025   36.3886
    9.3040    1.7281    7.1345   10.0815   25.4709   32.5571
   23.7039   16.1280    7.2654    4.3184   11.0710   18.1572
   34.7748   27.1989   18.3363   15.3893    0.0001    7.0863
   41.6866   34.1107   25.2481   22.3011    6.9117    0.1745
   53.2884   45.7125   36.8499   33.9029   18.5135   11.4273
   62.1595   54.5836   45.7210   42.7740   27.3846   20.2984
   66.2479   58.6720   49.8094   46.8624   31.4730   24.3868
  Columns 7 through 9
   61.9129   78.9981   87.4626
   57.1864   74.2716   82.7360
   53.2505   70.3357   78.8002
   47.8171   64.9023   73.3667
   43.9855   61.0707   69.5352
   29.5856   46.6708   55.1353
   18.5147   35.5999   44.0644
   11.6030   28.6881   37.1526
    0.0011   17.0863   25.5508
    8.8700    8.2152   16.6797
   12.9583    4.1268   12.5913
>> outpermone
outpermone =
  Columns 1 through 11
     1     2    12     3    13    14    15     4     6    16     5
  Columns 12 through 20
    17     9     8    18     7    10    19    11    20
>> outpermtwo
outpermtwo =
  Columns 1 through 11
     2     3    20     1    10    13     9    19    12     8    11
  Columns 12 through 20
    14     6    18     4    15     5     7    16    17
>> rowpermone'
ans =
     1     2     3     4     6     5     9     8     7    10    11
>> colpermone'
ans =
     1     2     3     4     5     6     7     8     9
>> rowpermtwo'
ans =
     2     3     1    10     9     8    11     6     4     5     7
>> colpermtwo'
ans =
     9     2     8     1     3     7     4     5     6
>> addconone
addconone =
  -57.7392
>> addcontwo
addcontwo =
   31.1328
>> coordone'
ans =
  Columns 1 through 6
         0   16.9587   17.1701   18.2499   25.8848   33.5284
  Columns 7 through 12
   45.6645   67.9306   79.6986   83.1923   85.0189  102.7361
  Columns 13 through 18
  128.0412  129.2524  131.6718  139.0949  139.1611  156.1808
  Columns 19 through 20
  169.8263  180.9922
>> coordtwo'
ans =
  Columns 1 through 6
         0    4.7265    8.6234    8.6624   14.0958   16.1993
  Columns 7 through 12
   17.9274   25.0619   28.0089   32.3273   43.3982   43.3983
  Columns 13 through 18
   50.3100   50.4845   61.9118   61.9129   70.7829   74.8713
  Columns 19 through 20
   78.9981   87.4626
>> axes'
ans =
  Columns 1 through 6
         0   16.9587   18.2499   67.9306   85.0189   79.6986
    8.6624         0    4.7265   61.9118   70.7829   50.3100
  Columns 7 through 12
  139.0949  129.2524  128.0412  139.1611  169.8263   17.1701
   74.8713   32.3273   17.9274   14.0958   43.3982   28.0089
  Columns 13 through 18
   25.8848   33.5284   45.6645   83.1923  102.7361  131.6718
   16.1993   43.3983   61.9129   78.9981   87.4626   50.4845
  Columns 19 through 20
  156.1808  180.9922
   25.0619    8.6234
```

4.4 Some Useful Two-Mode Utilities

This section gives several miscellaneous m-functions that carry out various operations on a two-mode proximity matrix, and for which no other section seemed appropriate. The first two, `proxstdtm.m` and `proxrandtm.m`, are very simple and provide standardized and randomly (entry-)permuted two-mode proximity matrices, respectively, that might be useful, for example, in testing the various m-functions we give. The syntax

```
[stanproxtm stanproxmulttm] = proxstdtm(proxtm,mean)
```

is intended to suggest that `STANPROXTM` provides a linear transformation of the entries in `PROXTM` to a standard deviation of one and a mean of `MEAN`; `STANPROXMULTTM` is a multiplicative transformation so the entries in this $n_a \times n_b$ matrix have a sum-of-squares of $n_a n_b$. For the second utility m-function

```
[randproxtm] = proxrandtm(proxtm)
```

implies that the two-mode matrix `RANDPROXTM` has its entries as a random permutation of the entries in `PROXTM`.

A third utility function, `proxmontm.m`, provides a monotonically transformed two-mode proximity matrix that is close in a least-squares sense to a given input two-mode matrix. The syntax is

```
[monproxpermuttm vaf diff] = proxmontm(proxpermuttm,fittedtm)
```

Here, `PROXPERMUTTM` is the original input two-mode proximity matrix (which may have been subjected to initial row and column permutations, hence the suffix '`PERMUTTM`'), and `FITTEDTM` is a given two-mode target matrix; the output matrix `MONPROXPERMUTTM` is closest to `FITTEDTM` in a least-squares sense and obeys the order constraints obtained from each pair of entries in `PROXPERMUTTM` (and where the inequality constrained optimization is carried out using the Dykstra-Kaczmarz iterative projection strategy); as usual, `VAF` denotes 'variance-accounted-for' and indicates how much variance in `MONPROXPERMUTTM` can be accounted for by `FITTEDTM`; finally, `DIFF` is the value of the least-squares loss function and is the sum of squared differences between the entries in `MONPROXPERMUTTM` and `FITTEDTM`. We will give an application of an m-file incorporating `proxmonton.m` when we suggest, in effect, a way of implementing two-dimensional, two-mode nonmetric multidimensional scaling in the next section.

A final utility function, `biplottm.m`, plots the combined row and column object set using the coordinates given in, for example, the $n \times 2$ output matrix `AXES` as output from the m-file of the last section, `biscaltmac.m`. The usage syntax is

```
 biplottm(axes,nrow,ncol)
```

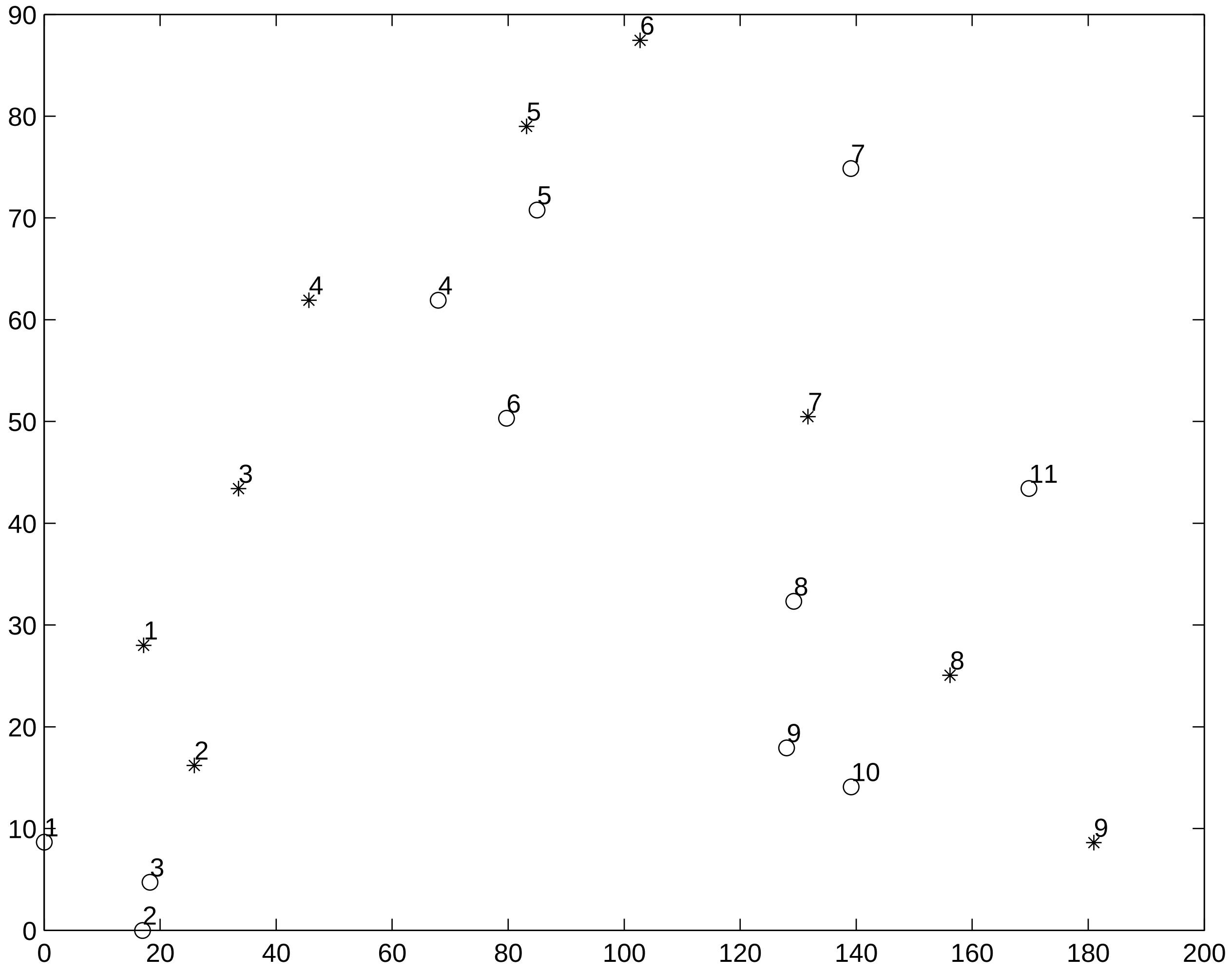

Figure 4.1: Two-dimensional joint biplot for the goldfish_receptor data obtained using biplottm.m

here the number of rows is `NROW` and the number of columns is `NCOL`, and n is the sum of `NROW` and `NCOL`. The first `NROW` rows of the $n \times 2$ matrix `AXES` give the row object coordinates; the last `NCOL` rows of `AXES` give the column object coordinates. The plotting symbol for rows is a circle (o); for columns it is an asterisk (*). The labels for rows are from 1 to `NROW`; those for columns are from 1 to `NCOL`.

Figure 4.1 give an application of `biplottm.m` for the `AXES` matrix of the last example given in section 4.3 (for the goldfish_receptor data). Again, the appropriate colors appear close to the relevant cones.

4.5 Two-mode Nonmetric Bidimensional Scaling

By uniting the utility function `proxmon.m` with `biscaltmac.m`, we can construct an m-file, `bimonscaltmac.m`, that carries out a nonmetric bidimensional scaling of a two-mode proximity matrix in the city-block metric. The usage is the same as that of `biscaltmac.m` in section 4.3, except for the additional output matrix `MONPROXTM` that is a monotonic transformation of the original two-mode proximity matrix `PROXTM`:

```
[..., monproxtm] = bimonscaltmac(...)
```

We give an example below using the same `goldfish_receptor.dat` matrix; the Vaf has increased to .9637. The joint plot of the row and column object set is given in Figure 4.2, and closely resembles Figure 4.1 obtained without the use of a monotonic transformation.

```
>> load goldfish_receptor.dat
>> goldfish_receptor

goldfish_receptor =

    47    53   111   143   188   196   200   200   200
    48    55    75   100   186   200   200   200   200
    46    47    90   125   168   176   177   183   200
    99   101    78    60    46    67   107   156   200
   122   127   115    79    49    46    91   143   200
   115   154    97    73    48   152    84   125   174
   198   186   154   148   103    94    63   108   155
   135   156   123   127   116    98    49    46    80
   141   113   142   148   114   121    61    47    54
   173   140   177   176   144   128    64    56    89
   200   200   160   161   145   138    80    53    68

>> [find,vaf,targone,targtwo,outpermone,outpermtwo, ...
  rowpermone,colpermone,rowpermtwo,colpermtwo,addconone,...
        addcontwo,coordone,coordtwo,axes,monproxtm] = ...
    bimonscaltmac(goldfish_receptor,1:20,1:20,1)

find =

  Columns 1 through 6

   93.3384   92.5173  113.0255  131.4652  170.2185  183.0480
   85.8901   93.5983  105.5771  124.0168  162.7702  175.5997
   92.3639   83.8293  103.9468  122.3865  161.1398  173.9693
  120.5688  122.8577  100.8818   83.8944   95.0878  107.9174
  135.5337  137.8225  115.8466   97.4069   80.1230   92.9525
  119.8908  122.1797  100.2038   97.5985   95.7658  108.5954
  170.9477  173.2365  151.2607  132.8210  103.6170   99.8346
  135.7153  138.0041  138.5364  139.6496  122.4090  118.6265
  136.8409  132.8759  141.8758  142.9890  125.7484  121.9659
  152.1182  143.5835  157.1531  158.2663  141.0257  137.2432
  174.7305  177.0193  155.0467  156.1599  138.9192  135.1367

  Columns 7 through 9

  177.8995  179.4117  195.4535
  170.4512  171.9634  193.6587
  168.8208  170.3330  186.3748
  111.9715  144.8897  169.6254
  107.5302  140.4483  165.1840
  103.4469  131.1856  155.9213
   86.3866  107.9264  132.6621
   87.6224   89.1346  113.8702
   92.7506   94.2628  110.5308
  101.1770   89.6770  105.7188
   99.0705   88.6572   97.3599


vaf =

    0.9637


targone =

  Columns 1 through 6

   19.2722   22.3951   26.5983   35.2615   63.2585   71.5645
   16.0886   19.2115   23.4146   32.0779   60.0749   68.3809
    4.0521    0.9292    3.2739   11.9372   39.9342   48.2402
   29.7693   26.6463   22.4432   13.7800   14.2170   22.5230
   36.2823   33.1594   28.9563   20.2930    7.7040   16.0100
   39.4723   36.3494   32.1463   23.4831    4.5139   12.8199
   64.3257   61.2028   56.9997   48.3364   20.3394   12.0334
   65.2201   62.0972   57.8940   49.2308   21.2338   12.9278
   73.4403   70.3174   66.1143   57.4510   29.4540   21.1480
   74.2572   71.1343   66.9312   58.2680   30.2710   21.9650
   92.9828   89.8599   85.6567   76.9935   48.9965   40.6905

  Columns 7 through 9

   87.0234  104.2385  124.6273
   83.8397  101.0549  121.4436
   63.6990   80.9142  101.3029
   37.9819   55.1970   75.5858
   31.4688   48.6840   69.0727
   28.2788   45.4940   65.8827
    3.4254   20.6406   41.0293
    2.5311   19.7462   40.1350
    5.6892   11.5260   31.9147
    6.5061   10.7091   31.0978
   25.2316    8.0165   12.3723


targtwo =

  Columns 1 through 6

   13.5118   15.6835   18.9235   20.0305   31.2845   35.7335
    3.0609    5.2326    8.4726    9.5796   20.8336   25.2826
    0.7338    1.4379    4.6779    5.7849   17.0389   21.4878
    2.2848    0.1131    3.1269    4.2339   15.4879   19.9368
    4.9985    2.8268    0.4132    1.5202   12.7742   17.2232
    6.5186    4.3469    1.1069    0.0001   11.2541   15.7030
   17.7711   15.5994   12.3594   11.2524    0.0016    4.4506
   19.6320   17.4602   14.2202   13.1132    1.8592    2.5897
   26.8230   24.6513   21.4113   20.3043    9.0503    4.6013
   32.0848   29.9130   26.6730   25.5660   14.3120    9.8631
   33.5308   31.3591   28.1191   27.0121   15.7581   11.3091

  Columns 7 through 9

   41.0610   51.8173   56.3408
   30.6101   41.3664   45.8899
   26.8153   37.5717   42.0952
   25.2643   36.0207   40.5442
   22.5507   33.3070   37.8305
   21.0305   31.7869   36.3104
```

```
    9.7781   20.5344   25.0579
    7.9172   18.6736   23.1971
    0.7262   11.4825   16.0060
    4.5356    6.2208   10.7443
    5.9817    4.7747    9.2982


outpermone =

  Columns 1 through 10

     1     2    12    13     3    14    15     4     6     5

  Columns 11 through 20

    16    17     9     8    18     7    10    19    11    20


outpermtwo =

  Columns 1 through 10

     3    10    13     1    20     9     2    12     8    19

  Columns 11 through 20

    11    14     6    18     4    15     5     7    16    17


rowpermone =

     1
     2
     3
     4
     6
     5
     9
     8
     7
    10
    11
```

```
colpermone =

     1
     2
     3
     4
     5
     6
     7
     8
     9


rowpermtwo =

     3
    10
     1
     9
     2
     8
    11
     6
     4
     5
     7


colpermtwo =

     2
     9
     1
     8
     3
     7
     4
     5
     6
```

```
addconone =

  -86.9484


addcontwo =

   17.5601


coordone =

         0
    3.1836
   19.2722
   22.3951
   23.3243
   26.5983
   35.2615
   49.0415
   55.5545
   58.7446
   63.2585
   71.5645
   83.5979
   84.4923
   87.0234
   92.7125
   93.5295
  104.2385
  112.2550
  124.6273


coordtwo =

         0
   10.4509
   13.5118
   14.2456
   15.6835
   15.7967
   18.5103
   18.9235
   20.0304
   20.0305
   31.2829
   31.2845
   33.1438
   35.7335
   40.3348
   41.0610
   45.5966
   47.0426
   51.8173
   56.3408


axes =

         0   14.2456
    3.1836   18.5103
   23.3243         0
   49.0415   40.3348
   58.7446   45.5966
   55.5545   33.1438
   92.7125   47.0426
   84.4923   20.0304
   83.5979   15.7967
   93.5295   10.4509
  112.2550   31.2829
   19.2722   18.9235
   22.3951   13.5118
   26.5983   31.2845
   35.2615   41.0610
   63.2585   51.8173
   71.5645   56.3408
   87.0234   35.7335
  104.2385   20.0305
  124.6273   15.6835


monproxtm =
  Columns 1 through 6

   88.5127   90.1385  114.8697  135.6526  173.2178  173.4785
   88.5127   91.3832   99.8841  114.8697  168.6422  177.2676
   88.5127   88.5127  104.0367  132.0685  157.3536  166.9333
  114.8697  114.8697   99.8841   91.3832   88.5127   99.8841
  132.0685  135.6526  122.9491   99.8841   88.5127   88.5127
  122.9491  135.6526  104.0367   99.8841   88.5127  135.6526
  173.4785  173.2178  141.0471  135.6526  114.8697  104.0367
  135.6526  141.0471  132.0685  135.6526  122.9491  114.8697
  135.6526  122.9491  135.6526  135.6526  122.9491  122.9491
  157.3536  135.6526  166.9333  159.4144  135.6526  135.6526
  176.3610  178.4635  155.9872  157.1575  135.6526  135.6526

  Columns 7 through 9

  179.8188  181.3929  198.0283
  173.4785  173.4785  195.7386
  168.6422  168.6422  188.4626
  114.8697  145.7035  173.4785
  104.0367  135.6526  173.4785
  104.0367  132.0685  157.3536
   91.3832  114.8697  141.0471
   88.5127   87.6897  104.0367
   91.3832   88.5127   91.3832
   99.8841   91.3832  104.0367
   99.8841   88.5127   99.8841
```

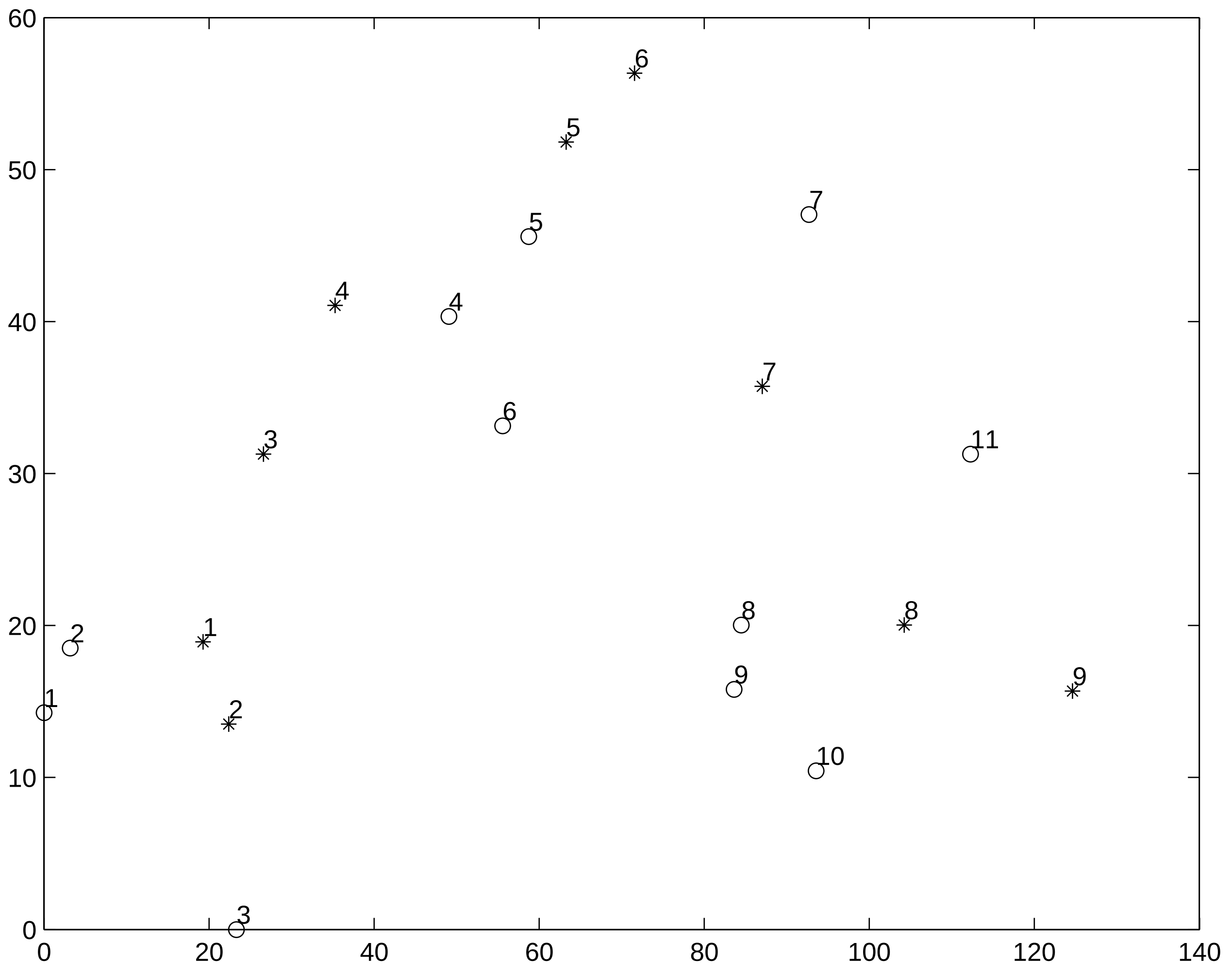

Figure 4.2: Two-dimensional joint biplot for the goldfish_receptor data obtained using bimonscaltmac.m and biplottm.m

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Part II

The Representation of Proximity Matrices by Tree Structures

Introduction to Graph-Theoretic Representational Structures

Various methods of data representation based on graph-theoretic structures have been developed over the last several decades for explaining the pattern of information potentially present in a single (or possibly, in a collection of) numerically given proximity matri(ces), each defined between pairs of objects from a single set, or in some cases, between the objects from several distinct sets (for example, see Carroll, 1976; Carroll, Clark, & DeSarbo, 1984; Carroll & Pruzansky, 1980; De Soete, 1983, 1984a,b,c; De Soete, Carroll, & DeSarbo, 1987; De Soete, DeSarbo, Furnas, & Carroll, 1984; Hutchinson, 1989; Klauer & Carroll, 1989, 1991; Hubert & Arabie, 1995). Typically, a specific class of graph-theoretic structures is assumed capable of representing the proximity information, and the proposed method seeks a member from the class producing a reconstructed set of proximities that are as close as possible to the original. The most prominent graph-theoretic structures used are those usually referred to as ultrametrics and additive trees, and these will be the primary emphasis here as well.

Although a variety of strategies have been proposed for locating good exemplars from whatever class of graph-theoretic structures is being considered, one approach has been to adopt a least squares criterion in which the class exemplar is identified by attempting to minimize the sum of squared discrepancies between the original proximities and their reconstructions obtained through the use of the particular structure selected by the data analyst. One common implementation of the least-squares optimization strategy has been defined by the usual least-squares criterion but augmented by some collection of penalty functions that seek to impose whatever constraints are mandated by the structural representation being sought. Then, through the use of some unconstrained optimization scheme (e.g., steepest descent, conjugate gradients), an attempt is made to find both (a) the particular constraints that should be imposed to define the specific structure from the class, and (b) the reconstructed proximities based on the structure finally identified. The resulting optimization strategy is heuristic in the sense that there is no guarantee of global optimality for the final structural representation identified even within the chosen graph-theoretic class, because the particular constraints defining the selected structure were located by a possibly reasonable but not verifiably optimal search strategy that was (implicitly) implemented in the course of the process of optimization. A second implementation of the least-squares optimization approach, and the one that we will concentrate on exclusively, is based on the type of iterative projection strategy already illustrated in conjunction with linear unidimensional scaling

(LUS) (see the addendum Section 1.4 on solving linear inequality constrained least-squares tasks), and developed in detail for the graph-theoretic context by Hubert and Arabie (1995). In its non-heuristic form, iterative projection allows the reconstruction of a set of proximities based on a fixed collection of constraints implied by whatever specific graph-theoretic structure has been selected for their representation. As in LUS, successive (or iterative) projections onto closed convex sets are carried out that are defined by the collection of given constraints implied by the structural representation chosen. Thus, the need for penalty terms is avoided and there is no explicit use of gradients in the attendant optimization strategy; also, it is fairly straightforward to incorporate a variety of different types of constraints that may be auxiliary to those generated from the given structural representation but none-the-less of interest to impose on the reconstruction.

As a least squares optimization strategy (in a non-heuristic form), iterative projection assumes that whatever constraint set is to be applied is completely known prior to its application. However, just as the various penalty-function and gradient-optimization techniques have been turned into heuristic search strategies for the particular structures of interest by allowing the collection of constraints to vary over the course of the optimization process, we attempt the same in using iterative projection to find the better-fitting ultrametrics and additive trees for a given proximity matrix. Thus, in addition to carrying out a least squares task subject to given structural constraints, iterative projection will be considered as one possible heuristic search strategy (and an alternative to those heuristic methods that have been suggested in the literature and based exclusively on the use of some type of penalty function) for locating the actual constraints to impose in the first instance, and therefore, to identify the general form of the structural representation sought.

The various least squares optimization tasks entailing both the identification of the specific form of the structural representation to adopt and the subsequent least squares fitting itself generally fall into the class of NP-hard problems (e.g., for ultrametric and additive trees, see Day, 1987; Kriválek, 1986; Kriválek & Moravek, 1986); thus, the best we can hope for is a heuristic extension of the iterative projection strategy leading to good but not necessarily optimal final structural representations within the general class of representations desired. As is standard with a reliance on such heuristic optimization methods, the use of multiple starting points will hopefully determine a set of local optima characterizing the better solutions attainable for a given data set. The presence of local optima in the use of any heuristic and combinatorially based optimization strategy is unavoidable, given the NP-hardness of the basic optimization tasks of interest and the general inability of (partial) enumeration methods (when available) to be computationally feasible for use on even moderate-sized data sets. The number of and variation in the local optima observable for any specific situation will obviously depend on the given data, the structural representation sought, and the heuristic search strategy used. But whenever present, local optima may actually be diagnostic for the structure(s) potentially appropriate for characterizing a particular data set. Thus, their identification may even be valuable in explaining the patterning of the data and/or in noting the difficulties with adopting a specific representational form to help discern underlying structure.

Chapter 5

Ultrametrics for Symmetric Proximity Data

The task of hierarchical clustering can be characterized as a specific data analysis problem: given a set of n objects, $S = \{O_1, \ldots, O_n\}$, and an $n \times n$ symmetric proximity matrix $\mathbf{P} = \{p_{ij}\}$ (nonnegative and with a dissimilarity interpretation), find a sequence of partitions of S, denoted as $\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_n$, satisfying the following:

(a) $\mathcal{P}_1$ is the (trivial) partition where all n objects from S are placed into n separate classes;

(b) $\mathcal{P}_n$ is the (also trivial) partition where a single subset contains all n objects;

(c) $\mathcal{P}_k$ is obtained from $\mathcal{P}_{k-1}$ by uniting some pair of classes present in $\mathcal{P}_{k-1}$;

(d) the minimum levels at which object pairs first appear together within the same class should reflect the proximities in $\mathcal{P}$. Or more formally, if we define $\mathbf{U}^0 = \{u^0_{ij}\} = \min\{k-1 \mid \text{objects } O_i \text{ and } O_j \text{ appear within the same class in the partition } \mathcal{P}_k\}$, then if the partition hierarchy is representing the given proximities well, the entries in $\mathbf{U}^0$ and $\mathbf{P}^0$ should be, for example, similarly ordered. We discuss the properties of matrices such as $\mathbf{U}^0$ in more detail below.

To give an example, we preformed a complete-link hierarchical clustering (using SYSTAT) on the `number.dat` proximity matrix used extensively in Part I, and obtained the following partitions of the object indices from 1 to 10 (remembering that these correspond to the digits 0 to 9):

$\mathcal{P}_1$: {{1},{2},{3},{4},{5},{6},{7},{8},{9},{10}}
$\mathcal{P}_2$: {{3,5},{1},{2},{4},{6},{7},{8},{9},{10}}
$\mathcal{P}_3$: {{3,5},{4,10},{1},{2},{6},{7},{8},{9}}
$\mathcal{P}_4$: {{3,5},{4,7,10},{1},{2},{6},{8},{9}}
$\mathcal{P}_5$: {{3,5,9},{4,7,10},{1},{2},{6},{8}}
$\mathcal{P}_6$: {{3,5,9},{4,7,10},{6,8},{1},{2}}
$\mathcal{P}_7$: {{3,5,9},{4,7,10},{6,8},{1,2}}
$\mathcal{P}_8$: {{3,5,9},{4,6,7,8,10},{1,2}}
$\mathcal{P}_9$: {{3,4,5,6,7,8,9,10},{1,2}}

$\mathcal{P}_{10}$: {{1,2,3,4,5,6,7,8,9,10}}

The matrix $\mathbf{U}^0$ was constructed and saved as a 10×10 matrix in the file `numcltarg.dat`, which will be used in an example later:

```
0 6 9 9 9 9 9 9 9 9
6 0 9 9 9 9 9 9 9 9
9 9 0 8 1 8 8 8 4 8
9 9 8 0 8 7 3 7 8 2
9 9 1 8 0 8 8 8 4 8
9 9 8 7 8 0 7 5 8 7
9 9 8 3 8 7 0 7 8 3
9 9 8 7 8 5 7 0 8 7
9 9 4 8 4 8 8 8 0 8
9 9 8 2 8 7 3 7 8 0
```

A concept routinely encountered in discussions of hierarchical clustering is that of an ultrametric, which can be characterized as any nonnegative symmetric dissimilarity matrix for the objects in S, denoted generically by $\mathbf{U} = \{u_{ij}\}$, where $u_{ij} = 0$ if and only if $i = j$, and $u_{ij} \leq \max[u_{ik}, u_{jk}]$ for all $1 \leq i, j, k \leq n$ (this last inequality is equivalent to the statement that for any distinct triple of subscripts, i, j, and k, the largest two proximities among u_{ij}, u_{ik}, and u_{jk} are equal and [therefore] not less than the third). Any ultrametric can be associated with the specific partition hierarchy it induces, having the form $\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_T$, where $\mathcal{P}_1$ and $\mathcal{P}_T$ are now the two trivial partitions that respectively contain all objects in separate classes and all objects in the same class, and $\mathcal{P}_k$ is formed from $\mathcal{P}_{k-1}$ ($2 \leq k \leq T$) by (agglomeratively) uniting certain (and possibly more than two) subsets in $\mathcal{P}_{k-1}$. For those subsets merged in $\mathcal{P}_{k-1}$ to form $\mathcal{P}_k$, all between-subset ultrametric values must be equal, and no less than any other ultrametric value associated with an object pair within a class in $\mathcal{P}_{k-1}$. Thus, individual partitions in the hierarchy can be identified by merely increasing a threshold variable starting at zero, and observing that $\mathcal{P}_k$ for $1 \leq k \leq T$ is defined by a set of subsets in which all within-subset ultrametric values are less than or equal to some specific threshold value, and all ultrametric values between subsets are strictly greater. Conversely, any partition hierarchy of the form $\mathcal{P}_1, \ldots, \mathcal{P}_T$ can be identified with the equivalence class of all ultrametric matrices that induce it. We note that if only a *single* pair of subsets can be united in $\mathcal{P}_{k-1}$ to form $\mathcal{P}_k$ for $2 \leq k \leq T$, then $T = n$, and we could then revert to the characterization of a full partition hierarchy $\mathcal{P}_1, \ldots, \mathcal{P}_n$ used earlier.

Given some fixed partition hierarchy $\mathcal{P}_1, \ldots, \mathcal{P}_T$, there are an infinite number of ultrametric matrices that induce it, but all can be generated by (restricted) monotonic functions of what might be called the basic ultrametric matrix $\mathbf{U}^0$ defined earlier. Explicitly, any ultrametric in the equivalence class whose members induce the same fixed hierarchy, $\mathcal{P}_1, \ldots, \mathcal{P}_T$, can be obtained by a strictly increasing monotonic function of the entries in $\mathbf{U}^0$, where the function maps zero to zero. Moreover, because u_{ij}^0 for $i \neq j$ can be only one of the integer values from 1 to $T - 1$, each ultrametric in the equivalence class that generates the fixed hierarchy may be defined by one of $T-1$ distinct values. When these $T-1$ values are ordered from the smallest to the largest, the $(k-1)^{st}$ smallest value corresponds to the partition $\mathcal{P}_k$ in the partition hierarchy $\mathcal{P}_1, \ldots, \mathcal{P}_T$, and implicitly to all object pairs that appear together for the first time within a subset in $\mathcal{P}_k$.

To provide an alternative interpretation, the basic ultrametric matrix can also be characterized as defining a collection of linear equality and inequality constraints that any ultrametric in a specific equivalence class must satisfy. Specifically, for each object triple there is (a) a specification of which ultrametric values among the three must be equal plus two additional inequality constraints so that the third is not greater; (b) an inequality or equality constraint for every pair of ultrametric values based on their order relationship in the basic ultrametric matrix; and (c) an equality constraint of zero for the main diagonal entries in $\mathbf{U}$. In any case, given these fixed equality and inequality constraints, standard L_p regression methods (such as those given in Späth, 1991, could be adapted to generate a best-fitting ultrametric, say $\mathbf{U}^* = \{u_{ij}^*\}$, to the given proximity matrix $\mathbf{P} = \{p_{ij}\}$. Concretely, we might find $\mathbf{U}^*$ by minimizing

$$\sum_{i<j}(p_{ij} - u_{ij})^2, \ \sum_{i<j} \mid p_{ij} - u_{ij} \mid, \text{ or possibly, } \max_{i<j} \mid p_{ij} - u_{ij} \mid .$$

(As a convenience here and later, it is assumed that $p_{ij} > 0$ for all $i \neq j$, to avoid the technicality of possibly locating best-fitting 'ultrametrics' that could violate the condition that $u_{ij} = 0$ if and only if $i = j$.)

5.1 Fitting a Given Ultrametric in the L_2 Norm

The MATLAB function, `ultrafit.m`, with usage

```
[fit,vaf] = ultrafit(prox,targ)
```

generates (using iterative projection based on the linear (in)equality constraints obtained from the fixed ultrametric — see Section 1.4) the best-fitting ultrametric in the L_2-norm (`FIT`) within the same equivalence class as that of a given ultrametric matrix `TARG`. The matrix `PROX` contains the symmetric input proximities and `VAF` is the variance-accounted-for (defined, as usual, by normalizing the obtained L_2-norm loss value:

$$\text{variance} - \text{accounted} - \text{for} = 1 - \frac{\sum_{i<j}(p_{ij} - u_{ij}^*)^2}{\sum_{i<j}(p_{ij} - \bar{p})^2},$$

where $\bar{p}$ is the mean off-diagonal proximity in $\mathbf{P}$, and $\mathbf{U}^* = \{u_{ij}^*\}$ is the best-fitting ultrametric.

In the example below, the target matrix is `numcltarg` obtained from the complete-link hierarchical clustering of `number`; the `VAF` generated by these ultrametric constraints is .4781. Comparing the target matrix `numcltarg` and `fit`, the particular monotonic function, say $f(\cdot)$, of the entries in the basic ultrametric matrix that generates the fitted matrix is: $f(1) =$ .0590, $f(2) =$ .2630, $f(3) =$ .2980, $f(4) =$ .3065, $f(5) =$ .4000, $f(6) =$ .4210, $f(7) =$ .4808, $f(8) =$ .5535, $f(9) =$ .6761.

```
load number.dat
load numcltarg.dat
[fit,vaf] = ultrafit(number,numcltarg)

fit =

  Columns 1 through 6

         0    0.4210    0.6761    0.6761    0.6761    0.6761
    0.4210         0    0.6761    0.6761    0.6761    0.6761
    0.6761    0.6761         0    0.5535    0.0590    0.5535
    0.6761    0.6761    0.5535         0    0.5535    0.4808
    0.6761    0.6761    0.0590    0.5535         0    0.5535
    0.6761    0.6761    0.5535    0.4808    0.5535         0
    0.6761    0.6761    0.5535    0.2980    0.5535    0.4808
    0.6761    0.6761    0.5535    0.4808    0.5535    0.4000
    0.6761    0.6761    0.3065    0.5535    0.3065    0.5535
    0.6761    0.6761    0.5535    0.2630    0.5535    0.4808

  Columns 7 through 10

    0.6761    0.6761    0.6761    0.6761
    0.6761    0.6761    0.6761    0.6761
    0.5535    0.5535    0.3065    0.5535
    0.2980    0.4808    0.5535    0.2630
    0.5535    0.5535    0.3065    0.5535
    0.4808    0.4000    0.5535    0.4808
         0    0.4808    0.5535    0.2980
    0.4808         0    0.5535    0.4808
    0.5535    0.5535         0    0.5535
    0.2980    0.4808    0.5535         0


vaf =

    0.4781
```

5.2 Finding an Ultrametric in the L_2 Norm

The m-file, `ultrafnd.m`, implements a heuristic search strategy using iterative projection to locate a best-fitting ultrametric in the L_2-norm. The method used is from Hubert and Arabie (1995); this latter source should be consulted for the explicit algorithmic details implemented in `ultrafnd.m` (as well as for many of the other m-files to be presented). The m-file usage has the form

```
[find,vaf] = ultrafnd(prox,inperm)
```

where `FIND` is the ultrametric identified having variance-accounted-for `VAF`. The matrix `PROX` contains the symmetric input proximities; `INPERM` is a permutation that defines an order in which the constraints are considered over all object triples. In the example below, for instance, `INPERM` is simply set as the MATLAB built-in random permutation function `randperm(n)` (using the size $n = 10$ explicitly for the `number` illustration). Thus, the search can be rerun with the same specification but now using a different random starting sequence. Two such searches are shown below leading to vafs of .4941 and .4781 (the latter is the same as obtained from fitting the best ultrametric in Section 5.1 using `numcltarg` for a fixed set of constraints; the former provides a slightly different and better-fitting ultrametric).

```
[find,vaf] = ultrafnd(number,randperm(10))

find =

  Columns 1 through 6

         0    0.7300    0.7300    0.7300    0.7300    0.7300
    0.7300         0    0.5835    0.5835    0.5835    0.5835
    0.7300    0.5835         0    0.5535    0.0590    0.5535
    0.7300    0.5835    0.5535         0    0.5535    0.4808
    0.7300    0.5835    0.0590    0.5535         0    0.5535
    0.7300    0.5835    0.5535    0.4808    0.5535         0
    0.7300    0.5835    0.5535    0.2980    0.5535    0.4808
    0.7300    0.5835    0.5535    0.4808    0.5535    0.4000
    0.7300    0.5835    0.3065    0.5535    0.3065    0.5535
    0.7300    0.5835    0.5535    0.2630    0.5535    0.4808

  Columns 7 through 10

    0.7300    0.7300    0.7300    0.7300
    0.5835    0.5835    0.5835    0.5835
    0.5535    0.5535    0.3065    0.5535
    0.2980    0.4808    0.5535    0.2630
    0.5535    0.5535    0.3065    0.5535
    0.4808    0.4000    0.5535    0.4808
         0    0.4808    0.5535    0.2980
    0.4808         0    0.5535    0.4808
    0.5535    0.5535         0    0.5535
    0.2980    0.4808    0.5535         0


vaf =

    0.4941

[find,vaf] = ultrafnd(number,randperm(10))

find =

  Columns 1 through 6

         0    0.4210    0.6761    0.6761    0.6761    0.6761
    0.4210         0    0.6761    0.6761    0.6761    0.6761
    0.6761    0.6761         0    0.5535    0.0590    0.5535
    0.6761    0.6761    0.5535         0    0.5535    0.4808
    0.6761    0.6761    0.0590    0.5535         0    0.5535
    0.6761    0.6761    0.5535    0.4808    0.5535         0
    0.6761    0.6761    0.5535    0.2980    0.5535    0.4808
    0.6761    0.6761    0.5535    0.4808    0.5535    0.4000
    0.6761    0.6761    0.3065    0.5535    0.3065    0.5535
    0.6761    0.6761    0.5535    0.2630    0.5535    0.4808

  Columns 7 through 10

    0.6761    0.6761    0.6761    0.6761
    0.6761    0.6761    0.6761    0.6761
    0.5535    0.5535    0.3065    0.5535
    0.2980    0.4808    0.5535    0.2630
    0.5535    0.5535    0.3065    0.5535
    0.4808    0.4000    0.5535    0.4808
         0    0.4808    0.5535    0.2980
    0.4808         0    0.5535    0.4808
    0.5535    0.5535         0    0.5535
    0.2980    0.4808    0.5535         0


vaf =

    0.4781
```

5.3 Representing an Ultrametric (Graphically)

Once an ultrametric matrix has been identified, there are two common ways in which the information within the matrix might be displayed. The first is to perform a simple reordering of the rows and columns of the given matrix to make apparent the sequence of partitions being induced by the ultrametric. The form desired is typically called anti-Robinson (see, for example, Hubert and Arabie, 1994, for a very complete discussion of using and fitting such matrix orderings). When a matrix is in anti-Robinson form, the entries within each row (and column) are non-decreasing moving away from the main diagonal in either direction. As the example given below will show, any ultrametric matrix can be put into such a form easily (and nonuniquely). The second strategy for representing an ultrametric relies on the graphical form of a tree (or as it is typically called in the classification literature, a dendrogram), and where one can read the values of the ultrametric directly from the displayed structure. We give an example of such a tree below (and provide at the end of this Chapter the LaTeX code [within the `picture` environment] to generate this particular graphical structure).

To give the illustration of reordering an ultrametric matrix to display its anti-Robinson form, the example found in Section 5.2 with a vaf of .4941 will be used, along with a short m-file, `ultraorder.m`. This function implements a simple mechanism of first generating a unidimensional equally-spaced target matrix from the utility m-file `ransymat.m`, and then re-orders heuristically the given ultrametric matrix against this given target with the quadratic assignment functions `pairwiseqa.m` and `insertqa.m` (the latter uses a block size of 1 for `kblock`). The explicit usage is

```
[orderprox,orderperm] = ultraorder(prox)
```

where `PROX` is a supposedly ultrametric matrix; `ORDERPERM` is a permutation used to display the anti-Robinson form in `ORDERPROX` where `orderprox = prox(orderperm,orderperm)`.

```
load number.dat
[find,vaf] = ultrafnd(number,randperm(10))

find =

  Columns 1 through 6

         0    0.7300    0.7300    0.7300    0.7300    0.7300
    0.7300         0    0.5835    0.5835    0.5835    0.5835
    0.7300    0.5835         0    0.5535    0.0590    0.5535
    0.7300    0.5835    0.5535         0    0.5535    0.4808
    0.7300    0.5835    0.0590    0.5535         0    0.5535
    0.7300    0.5835    0.5535    0.4808    0.5535         0
    0.7300    0.5835    0.5535    0.2980    0.5535    0.4808
    0.7300    0.5835    0.5535    0.4808    0.5535    0.4000
    0.7300    0.5835    0.3065    0.5535    0.3065    0.5535
    0.7300    0.5835    0.5535    0.2630    0.5535    0.4808

  Columns 7 through 10

    0.7300    0.7300    0.7300    0.7300
    0.5835    0.5835    0.5835    0.5835
    0.5535    0.5535    0.3065    0.5535
    0.2980    0.4808    0.5535    0.2630
    0.5535    0.5535    0.3065    0.5535
    0.4808    0.4000    0.5535    0.4808
         0    0.4808    0.5535    0.2980
    0.4808         0    0.5535    0.4808
    0.5535    0.5535         0    0.5535
    0.2980    0.4808    0.5535         0


vaf =

    0.4941

[orderprox,orderperm] = ultraorder(find)

orderprox =

  Columns 1 through 6

         0    0.7300    0.7300    0.7300    0.7300    0.7300
    0.7300         0    0.3065    0.3065    0.5535    0.5535
    0.7300    0.3065         0    0.0590    0.5535    0.5535
    0.7300    0.3065    0.0590         0    0.5535    0.5535
    0.7300    0.5535    0.5535    0.5535         0    0.2630
    0.7300    0.5535    0.5535    0.5535    0.2630         0
    0.7300    0.5535    0.5535    0.5535    0.2980    0.2980
    0.7300    0.5535    0.5535    0.5535    0.4808    0.4808
    0.7300    0.5535    0.5535    0.5535    0.4808    0.4808
    0.7300    0.5835    0.5835    0.5835    0.5835    0.5835

  Columns 7 through 10

    0.7300    0.7300    0.7300    0.7300
    0.5535    0.5535    0.5535    0.5835
    0.5535    0.5535    0.5535    0.5835
    0.5535    0.5535    0.5535    0.5835
    0.2980    0.4808    0.4808    0.5835
    0.2980    0.4808    0.4808    0.5835
         0    0.4808    0.4808    0.5835
    0.4808         0    0.4000    0.5835
    0.4808    0.4000         0    0.5835
    0.5835    0.5835    0.5835         0


orderperm =

     1     9     3     5    10     4     7     8     6     2
```

The reordered matrix using the row and column order of $0 \prec 8 \prec 2 \prec 4 \prec 9 \prec 3 \prec 6 \prec 7 \prec 5 \prec 1$ is given below; here the blocks of equal-valued entries are highlighted, indicating the partition hierarchy (also given below) induced by the ultrametric.

	0	8	2	4	9	3	6	7	5	1
0	x	.73	.73	.73	.73	.73	.73	.73	.73	.73
8	.73	x	.31	.31	.55	.55	.55	.55	.55	.58
2	.73	.31	x	.06	.55	.55	.55	.55	.55	.58
4	.73	.31	.06	x	.55	.55	.55	.55	.55	.58
9	.73	.55	.55	.55	x	.26	.30	.48	.48	.58
3	.73	.55	.55	.55	.26	x	.30	.48	.48	.58
6	.73	.55	.55	.55	.30	.30	x	.48	.48	.58
7	.73	.55	.55	.55	.48	.48	.48	x	.40	.58
5	.73	.55	.55	.55	.48	.48	.48	.40	x	.58
1	.73	.58	.58	.58	.58	.58	.58	.58	.58	x

Partition	Level Formed
{{0,8,2,4,9,3,6,7,5,1}}	.73
{{0},{8,2,4,9,3,6,7,5,1}}	.58
{{0},{8,2,4,9,3,6,7,5},{1}}	.55
{{0},{8,2,4},{9,3,6,7,5},{1}}	.48
{{0},{8,2,4},{9,3,6},{7,5},{1}}	.40
{{0},{8,2,4},{9,3,6},{7},{5},{1}}	.31
{{0},{8},{2,4},{9,3,6},{7},{5},{1}}	.30
{{0},{8},{2,4},{9,3},{6},{7},{5},{1}}	.26
{{0},{8},{2,4},{9},{3},{6},{7},{5},{1}}	.06
{{0},{8},{2},{4},{9},{3},{6},{7},{5},{1}}	—

For the partition hierarchy just given, the alternative structure of a dendrogram (or tree) for its representation is given in the figure that follows. The terminal "nodes" of this structure, indicated by open circles, correspond to the ten digits; the filled circles are internal "nodes" reflecting the level at which certain new classes in a partition hierarchy are constructed. For instance, using the calibration given on the long vertical line at the left, a new class consisting of the digits {9,3,6,7,5} is formed at level .48 by uniting the two classes {9,3,6} and {7,5}. Thus, in the ultrametric matrix given earlier, the values between the entries in these two classes are all a constant .48.

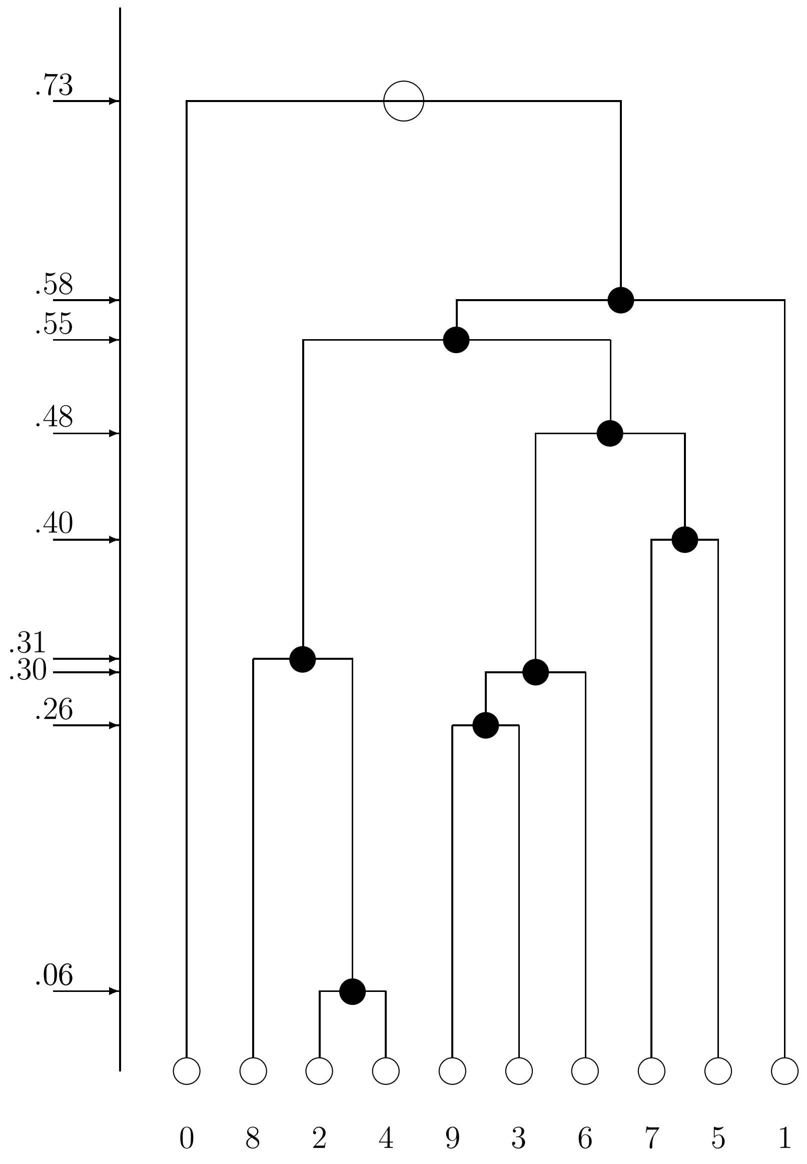
The dendrogram just given can be modified (or at least in how it should be interpreted) to motivate the representational form of an additive tree to be introduced in Chapter 6: (a) the values in the calibration along the long vertical axis need to be cut in half; (b) all horizontal lines are now to be understood as having no length and are present only for graphical convenience; (c) a spot on the dendrogram is indicated (here, by a large open circle), called the "root". A crucial characterization feature of an ultrametric is that the root is equidistant from all terminal nodes.

Given these interpretive changes, the ultrametric values for each object pair can now be reconstructed by the length of the path in the tree connecting the two relevant objects. Thus, an ultrametric is reconstructed from the lengths of paths between objects in a tree; and the special form of a tree for an ultrametric is one in which there exists a root that is equidistant from all terminal nodes. In the generalization to an additive tree of Chapter 6, the condition of requiring the existence of an equidistant root is removed, which amounts to allowing the branches attached to the terminal nodes to be stretched or shrunk at will.

5.3.1 LaTeX Code for the Dendrogram of Figure 5.1

```
\begin{figure}

\caption{A Dendrogram (Tree) Representation for the
Ultrametric Described in the Text Having Vaf of .4941}

\setlength{\unitlength}{.5pt}

\begin{picture}(500,1000)

\put(50,0){\makebox(0,0){0}}
\put(100,0){\makebox(0,0){8}}
\put(150,0){\makebox(0,0){2}}
\put(200,0){\makebox(0,0){4}}
\put(250,0){\makebox(0,0){9}}
\put(300,0){\makebox(0,0){3}}
\put(350,0){\makebox(0,0){6}}
```

Figure 5.1: A Dendrogram (Tree) Representation for the Ultrametric Described in the Text Having Vaf of .4941



```
\put(400,0){\makebox(0,0){7}}
\put(450,0){\makebox(0,0){5}}
\put(500,0){\makebox(0,0){1}}


\put(50,50){\circle{20}}
\put(100,50){\circle{20}}
\put(150,50){\circle{20}}
\put(200,50){\circle{20}}
\put(250,50){\circle{20}}
\put(300,50){\circle{20}}
\put(350,50){\circle{20}}
\put(400,50){\circle{20}}
\put(450,50){\circle{20}}
\put(500,50){\circle{20}}

\put(175,110){\circle*{20}}
\put(275,310){\circle*{20}}
\put(312.5,350){\circle*{20}}
\put(137.5,360){\circle*{20}}
\put(425,450){\circle*{20}}
\put(368.75,530){\circle*{20}}
\put(253.125,600){\circle*{20}}
\put(376.5625,630){\circle*{20}}
\put(213.28125,780){\circle{30}}

\put(0,50){\line(0,1){800}}
\put(50,60){\line(0,1){720}}
\put(100,60){\line(0,1){300}}
\put(150,60){\line(0,1){50}}
\put(200,60){\line(0,1){50}}
\put(250,60){\line(0,1){250}}
\put(300,60){\line(0,1){250}}
\put(350,60){\line(0,1){290}}
\put(400,60){\line(0,1){390}}
\put(450,60){\line(0,1){390}}
\put(500,60){\line(0,1){570}}
\put(175,110){\line(0,1){250}}
\put(275,310){\line(0,1){40}}
\put(312.5,350){\line(0,1){180}}
\put(425,450){\line(0,1){80}}
\put(368.75,530){\line(0,1){70}}
```

```
\put(137.5,360){\line(0,1){240}}
\put(253.125,600){\line(0,1){30}}
\put(376.5625,630){\line(0,1){150}}

\put(150,110){\line(1,0){50}}
\put(250,310){\line(1,0){50}}
\put(275,350){\line(1,0){75}}
\put(100,360){\line(1,0){75}}
\put(400,450){\line(1,0){50}}
\put(312.5,530){\line(1,0){112.5}}
\put(137.5,600){\line(1,0){231.25}}
\put(253.125,630){\line(1,0){246.875}}
\put(50,780){\line(1,0){326.5625}}

\put(-50,110){\vector(1,0){50}}
\put(-50,115){\makebox(0,0)[b]{.06}}
\put(-50,310){\vector(1,0){50}}
\put(-50,315){\makebox(0,0)[b]{.26}}
\put(-50,350){\vector(1,0){50}}
\put(-70,345){\makebox(0,0)[b]{.30}}
\put(-50,360){\vector(1,0){50}}
\put(-70,365){\makebox(0,0)[b]{.31}}
\put(-50,450){\vector(1,0){50}}
\put(-50,455){\makebox(0,0)[b]{.40}}
\put(-50,530){\vector(1,0){50}}
\put(-50,535){\makebox(0,0)[b]{.48}}
\put(-50,600){\vector(1,0){50}}
\put(-50,605){\makebox(0,0)[b]{.55}}
\put(-50,630){\vector(1,0){50}}
\put(-50,635){\makebox(0,0)[b]{.58}}
\put(-50,780){\vector(1,0){50}}
\put(-50,785){\makebox(0,0)[b]{.73}}
\put(-50,110){\vector(1,0){50}}
\put(-50,115){\makebox(0,0)[b]{.06}}

\end{picture}
\end{figure}
```

5.3.2 Plotting the Dendrogram with ultraplot.m

The m-file, `ultraplot.m`, uses several of the routines in the MATLAB Statistics Toolbox to plot the dendrogram associated with an ultrametric matrix. So, if the user has the latter

Toolbox available, a graphical representation of the ultrametric can be generated directly with the syntax

```
ultraplot(ultra)
```

where `ULTRA` is the ultrametric matrix. A figure window opens in MATLAB displaying the appropriate tree, which can then be saved in, say, an encapsulated postscript form and included in a printed document. The example below is how the tree looks obtained from `number.dat` and `ultrafnd.m`.

```
>> load number.dat
>> [find,vaf] = ultrafnd(number,randperm(10));


vaf =

    0.4941

>> ultraplot(find)

additive_constant =

     0
```

If there are any negative values in the input matrix `ultra` (as obtained, for example, when fitting multiple ultrametrics to a single proximity matrix), an additive_constant equal to the negative of the minimum value in `ultra` is added to the off-diagonal entries in `ultra` before the plot is carried out.

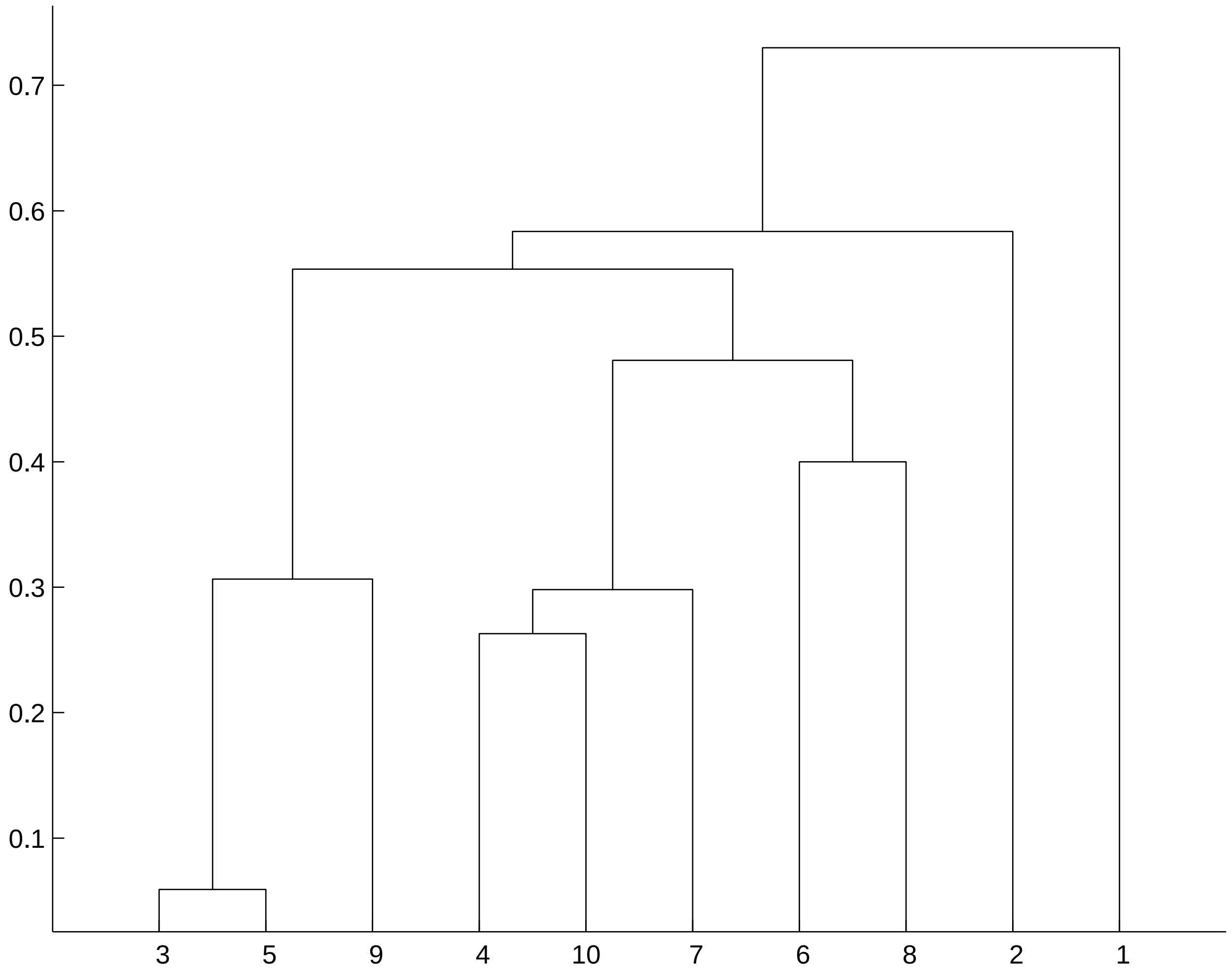


Figure 5.2: Dendrogram plot for the number.dat data obtained using ultraplot.m

Chapter 6

Additive Trees for Symmetric Proximity Data

A currently popular alternative to the use of a simple ultrametric in classification, and which might be considered a natural extension of the notion of an ultrametric, is that of an additive tree; comprehensive discussions can be found in Mirkin (1996, Chapter 7) or throughout Barthélemy and Guénoche (1991). Generalizing the earlier characterization of an ultrametric, an $n \times n$ matrix $\mathbf{A} = \{a_{ij}\}$ can be called an additive tree (metric or matrix) if the three-object (or three-point) ultrametric condition is replaced by a four-object (or four-point) condition: $a_{ij} + a_{kl} \leq \max\{a_{ik} + a_{jl}, a_{il} + a_{jk}\}$ for $1 \leq i, j, k, l \leq n$; equivalently, for any object quadruple O_i, O_j, O_k, and O_l, the largest two values among the sums $a_{ij} + a_{kl}$, $a_{ik} + a_{jl}$, and $a_{il} + a_{jk}$ must be equal.

Any additive tree matrix $\mathbf{A}$ can be represented (in many ways) as a sum of two matrices, say $\mathbf{U} = \{u_{ij}\}$ and $\mathbf{C} = \{c_{ij}\}$, where $\mathbf{U}$ is an ultrametric matrix, and $c_{ij} = g_i + g_j$ for $1 \leq i \neq j \leq n$ and $c_{ii} = 0$ for $1 \leq i \leq n$, based on some set of values $g_1, \ldots, g_n$. The multiplicity of such possible decompositions results from the choice of where to essentially place the root in the type of graphical tree representation we will generally use. Generally, for us, the root will be placed half-way along the longest path in the tree, generating a decomposition of the matrix $\mathbf{A}$ using a procedure from Barthélemy and Guénoche (1991, Section 3.3.3):

(a) Given $\mathbf{A}$, let $O_{i*}, O_{j*} \in S$ denote the two objects between which the longest path is defined in the tree, i.e., the pair of objects O_{i*} and O_{j*} is associated with the largest entry in $\mathbf{A}$, say a_{i*j*}.

(b) Define $\mathbf{U}$ by letting

$$u_{ij} = a_{ij} - (g_i + g_j), \text{ where } g_i = \max\{a_{ii*}, a_{jj*}\} - M,$$

with M chosen so that $u_{ij} > 0$ for $i \neq j$. The matrix $\mathbf{C} = \{c_{ij}\}$ is then constructed by letting $c_{ii} = 0$ for $1 \leq i \leq n$, and $c_{ij} = g_i + g_j$ for $1 \leq i \neq j \leq n$. (If M is set equal to the largest entry a_{i*j*}, the values in $\mathbf{U}$ would have to be positive, and two values among $g_1, \ldots, g_n$ would be zero with the remainder less than or equal to zero. Thus, a value for M

less than a_{i*j*} is usually found by trial-and-error that will give positive entries within $\mathbf{U}$ and as many positive values as possible for $g_1, \ldots, g_n$.)

To construct the type of graphical additive tree representation we will give below, the process followed is to first graph the dendrogram induced by $\mathbf{U}$, where (as for any ultrametric) the chosen root is equidistant from all terminal nodes. The branches connecting the terminal nodes are then lengthened or shortened depending on the signs and absolute magnitudes of $g_1, \ldots, g_n$. If one were willing to consider the (arbitrary) inclusion of a sufficiently large additive constant to the entries of $\mathbf{A}$, the values of $g_1, \ldots, g_n$ could be assumed non-negative. In this case, the matrix $\mathbf{C}$ would represent what is now commonly called a centroid metric (see, for example, the usage in Barthélemy and Guénoche, 1991, Chapter 3); although having some advantages (particularly for some of the graphical representations we give in avoiding the issue of presenting negative branch lengths), such a restriction is not absolutely necessary for what we do in the sequel. In fact, even though some of the entries among $g_1, \ldots, g_n$ may be negative, for convenience we will still routinely refer to a centroid metric (component) even though some of the defined "distances" may actually be negative.

6.1 Fitting a Given Additive Tree in the L_2 Norm

The MATLAB function, `atreefit.m`, with usage

```
[fit,vaf] = atreefit(prox,targ)
```

parallels that of `ultrafit.m` of Section 5.1; it generates (again using iterative projection based on the linear (in)equality constraints obtained from a fixed additive tree — see Section 1.4) the best-fitting additive tree in the L_2-norm (`FIT`) within the same equivalence class as that of a given additive tree matrix `TARG`. The matrix `PROX` contains the symmetric input proximities and `VAF` is the variance-accounted-for.

In the example below, the target matrix is again `numcltarg` obtained from the complete-link hierarchical clustering of `number.dat`; the `VAF` generated by these (now considered as additive tree) constraints is .6249 (and, as to be expected, is a value larger than for the corresponding best-fitting ultrametric value of .4781).

```
[fit,vaf] = atreefit(number,numcltarg)


fit =


  Columns 1 through 6

         0    0.4210    0.7185    0.7371    0.7092    0.8188
    0.4210         0    0.5334    0.5520    0.5241    0.6337
    0.7185    0.5334         0    0.4882    0.0590    0.5700
    0.7371    0.5520    0.4882         0    0.4790    0.4337
    0.7092    0.5241    0.0590    0.4790         0    0.5607
    0.8188    0.6337    0.5700    0.4337    0.5607         0
    0.7116    0.5265    0.4627    0.2506    0.4535    0.4082
    0.8670    0.6818    0.6181    0.4818    0.6089    0.4000
    0.7549    0.5698    0.3111    0.5247    0.3019    0.6064
    0.8318    0.6467    0.5830    0.2630    0.5737    0.5284

  Columns 7 through 10

    0.7116    0.8670    0.7549    0.8318
    0.5265    0.6818    0.5698    0.6467
    0.4627    0.6181    0.3111    0.5830
    0.2506    0.4818    0.5247    0.2630
    0.4535    0.6089    0.3019    0.5737
    0.4082    0.4000    0.6064    0.5284
         0    0.4563    0.4992    0.3454
    0.4563         0    0.6546    0.5766
    0.4992    0.6546         0    0.6194
    0.3454    0.5766    0.6194         0

vaf =

    0.6249
```

6.2 Finding an Additive Tree in the L_2 Norm

In analogy to the m-file, `ultrafnd.m`, from Section 5.2 for identifying best-fitting ultrametrics, `atreefnd.m` implements the Hubert and Arabie (1995) heuristic search strategy using iterative projection but now for constructing the best-fitting additive trees in the L_2-norm. The usage has the form

```
[find,vaf] = atreefnd(prox,inperm)
```

where `FIND` is the identified additive tree with variance-accounted-for `VAF`. Again, the matrix `PROX` contains the symmetric input proximities, and `INPERM` is a permutation that defines an order in which the constraints are considered over all object quadruples. In the example below, two such searches are shown starting with random permutations (through the use of `randperm(10)`) that give vafs of .6359 and .6249.

```
[find,vaf] = atreefnd(number,randperm(10))

find =

  Columns 1 through 6
```

```
         0    0.4210    0.6467    0.6448    0.6374    0.8049
    0.4210         0    0.4616    0.4596    0.4523    0.6198
    0.6467    0.4616         0    0.3634    0.0590    0.5235
    0.6448    0.4596    0.3634         0    0.3542    0.4385
    0.6374    0.4523    0.0590    0.3542         0    0.5143
    0.8049    0.6198    0.5235    0.4385    0.5143         0
    0.7523    0.5671    0.4709    0.3858    0.4617    0.4132
    0.9263    0.7412    0.6449    0.5599    0.6357    0.5872
    0.8634    0.6783    0.5820    0.4970    0.5728    0.5244
    0.8733    0.6881    0.5919    0.5068    0.5827    0.5342

  Columns 7 through 10

    0.7523    0.9263    0.8634    0.8733
    0.5671    0.7412    0.6783    0.6881
    0.4709    0.6449    0.5820    0.5919
    0.3858    0.5599    0.4970    0.5068
    0.4617    0.6357    0.5728    0.5827
    0.4132    0.5872    0.5244    0.5342
         0    0.3930    0.3301    0.3400
    0.3930         0    0.4000    0.4569
    0.3301    0.4000         0    0.3941
    0.3400    0.4569    0.3941         0

vaf =

    0.6359

[find,vaf] = atreefnd(number,randperm(10))

find =

  Columns 1 through 6

         0    0.4210    0.7185    0.7371    0.7092    0.8188
    0.4210         0    0.5334    0.5520    0.5241    0.6337
    0.7185    0.5334         0    0.4882    0.0590    0.5700
    0.7371    0.5520    0.4882         0    0.4790    0.4337
    0.7092    0.5241    0.0590    0.4790         0    0.5607
    0.8188    0.6337    0.5700    0.4337    0.5607         0
    0.7116    0.5265    0.4627    0.2506    0.4535    0.4082
    0.8670    0.6818    0.6181    0.4818    0.6089    0.4000
    0.7549    0.5698    0.3111    0.5247    0.3019    0.6064
    0.8318    0.6467    0.5830    0.2630    0.5737    0.5284

  Columns 7 through 10

    0.7116    0.8670    0.7549    0.8318
    0.5265    0.6818    0.5698    0.6467
    0.4627    0.6181    0.3111    0.5830
    0.2506    0.4818    0.5247    0.2630
    0.4535    0.6089    0.3019    0.5737
    0.4082    0.4000    0.6064    0.5284
         0    0.4563    0.4992    0.3454
    0.4563         0    0.6546    0.5766
    0.4992    0.6546         0    0.6194
    0.3454    0.5766    0.6194         0

vaf =

    0.6249
```

6.3 Decomposing an Additive Tree

The m-file, `atreedec.m`, decomposes a given additive tree matrix into an ultrametric and a centroid metric matrix (where the root is half-way along the longest path). The form of the usage is

```
[ulmetric,ctmetric] = atreedec(prox,constant)
```

where `PROX` is the input (additive tree) proximity matrix (with a zero main diagonal and a dissimilarity interpretation); `CONSTANT` is a nonnegative number (less than or equal to the maximum proximity value) that controls the positivity of the constructed ultrametric values; `ULMETRIC` is the ultrametric component of the decomposition; `CTMETRIC` is the centroid metric component (given by values $g_1, \ldots, g_n$ assigned to each of the objects, some of which may actually be negative depending on the input proximity matrix used). In the example below, the additive tree matrix identified earlier with a vaf of .6359, is decomposed using a value of .70 for the constant to control the positivity of the ultrametric values.

```
load number.dat
[find,vaf] = atreefnd(number,randperm(10))
```

```
find =

  Columns 1 through 7

         0    0.4210    0.6467    0.6448    0.6374    0.8049    0.7523
    0.4210         0    0.4616    0.4596    0.4523    0.6198    0.5671
    0.6467    0.4616         0    0.3634    0.0590    0.5235    0.4709
    0.6448    0.4596    0.3634         0    0.3542    0.4385    0.3858
    0.6374    0.4523    0.0590    0.3542         0    0.5143    0.4617
    0.8049    0.6198    0.5235    0.4385    0.5143         0    0.4132
    0.7523    0.5671    0.4709    0.3858    0.4617    0.4132         0
    0.9263    0.7412    0.6449    0.5599    0.6357    0.5872    0.3930
    0.8634    0.6783    0.5820    0.4970    0.5728    0.5244    0.3301
    0.8733    0.6881    0.5919    0.5068    0.5827    0.5342    0.3400

  Columns 8 through 10

    0.9263    0.8634    0.8733
    0.7412    0.6783    0.6881
    0.6449    0.5820    0.5919
    0.5599    0.4970    0.5068
    0.6357    0.5728    0.5827
    0.5872    0.5244    0.5342
    0.3930    0.3301    0.3400
         0    0.4000    0.4569
    0.4000         0    0.3941
    0.4569    0.3941         0


vaf =

    0.6359

[ulmetric,ctmetric] = atreedec(find,.70)

ulmetric =

  Columns 1 through 7

         0    0.1536    0.4737    0.4737    0.4737    0.4737    0.4737
    0.1536         0    0.4737    0.4737    0.4737    0.4737    0.4737
    0.4737    0.4737         0    0.4720    0.1749    0.4720    0.4720
    0.4737    0.4737    0.4720         0    0.4720    0.3888    0.3888
    0.4737    0.4737    0.1749    0.4720         0    0.4720    0.4720
    0.4737    0.4737    0.4720    0.3888    0.4720         0    0.2560
    0.4737    0.4737    0.4720    0.3888    0.4720    0.2560         0
    0.4737    0.4737    0.4720    0.3888    0.4720    0.2560    0.1144
    0.4737    0.4737    0.4720    0.3888    0.4720    0.2560    0.1144
    0.4737    0.4737    0.4720    0.3888    0.4720    0.2560    0.1144

  Columns 8 through 10

    0.4737    0.4737    0.4737
    0.4737    0.4737    0.4737
    0.4720    0.4720    0.4720
    0.3888    0.3888    0.3888
    0.4720    0.4720    0.4720
    0.2560    0.2560    0.2560
    0.1144    0.1144    0.1144
         0    0.0103    0.0574
    0.0103         0    0.0574
    0.0574    0.0574         0


ctmetric =

    0.2263
    0.0412
   -0.0533
   -0.0552
   -0.0626
    0.1049
    0.0523
    0.2263
    0.1634
    0.1733

[orderprox,orderperm] = ultraorder(ulmetric)


orderprox =

  Columns 1 through 7
```

```
         0    0.1536    0.4737    0.4737    0.4737    0.4737    0.4737
    0.1536         0    0.4737    0.4737    0.4737    0.4737    0.4737
    0.4737    0.4737         0    0.1749    0.4720    0.4720    0.4720
    0.4737    0.4737    0.1749         0    0.4720    0.4720    0.4720
    0.4737    0.4737    0.4720    0.4720         0    0.2560    0.2560
    0.4737    0.4737    0.4720    0.4720    0.2560         0    0.1144
    0.4737    0.4737    0.4720    0.4720    0.2560    0.1144         0
    0.4737    0.4737    0.4720    0.4720    0.2560    0.1144    0.0574
    0.4737    0.4737    0.4720    0.4720    0.2560    0.1144    0.0574
    0.4737    0.4737    0.4720    0.4720    0.3888    0.3888    0.3888

  Columns 8 through 10

    0.4737    0.4737    0.4737
    0.4737    0.4737    0.4737
    0.4720    0.4720    0.4720
    0.4720    0.4720    0.4720
    0.2560    0.2560    0.3888
    0.1144    0.1144    0.3888
    0.0574    0.0574    0.3888
         0    0.0103    0.3888
    0.0103         0    0.3888
    0.3888    0.3888         0


orderperm =

     2     1     3     5     6     7    10     9     8     4
```

6.4 Representing an Additive Tree (Graphically)

The information present in an additive tree can be provided in several ways. First, given the decomposition into an ultrametric and a centroid metric, the partition hierarchy induced by the ultrametric could be given explicitly, along with the levels at which the various new subsets in the partitions are formed. The fitted additive tree values could then be identified as a sum of (a) the level at which an object pair, say O_i and O_j, first appear together within a common subset of the hierarchy, and (b) the sum of g_i and g_j for the pair from the centroid metric component. As an illustration using the example just given in Section 6.3, the partition hierarchy has the form:

Partition	Level Formed
{{1,0,2,4,5,6,9,8,7,3}}	.47
{{1,0},{2,4},{5,6,9,8,7,3}}	.39
{{1,0},{2,4},{5,6,9,8,7},{3}}	.26
{{1,0},{2,4},{5},{6,9,8,7},{3}}	.17
{{1,0},{2},{4},{5},{6,9,8,7},{3}}	.15
{{1},{0},{2},{4},{5},{6,9,8,7},{3}}	.11
{{1},{0},{2},{4},{5},{6},{9,8,7},{3}}	.06
{{1},{0},{2},{4},{5},{6},{9},{8,7},{3}}	.01
{{1},{0},{2},{4},{5},{6},{9},{8},{7},{3}}	.00

with centroid metric values of:

digit	g_i
0	.23
1	.04
2	-.05
3	-.06
4	-.06
5	.10
6	.05
7	.23
8	.16
9	.17

Thus, the additive tree value for the digit pair (3,6) of .39 [.3858] is formed from the level .39 [.3888] at which 3 and 6 first appear together in the hierarchy, plus the sum of the g_is for the two digits of -.06 [-.0552] and .05 [.0523]. A dendrogram representation for the partition hierarchy is given in Figure 6.1.

A graphical representation for the additive tree is given in Figure 6.2 which was obtained from the dendrogram of Figure 6.1 by stretching and shrinking the branches attached to the terminal nodes by the g_i values (and cutting the vertical scale given in the dendrogram by half). Thus, the length of a path in the tree from one terminal node to another (ignoring all horizontal lines as having lengths of zero), would generate the values given in the additive tree matrix. The LaTeXcode to construct Figures 6.2 and 6.3 is given at the end of this section.

6.4.1 The LaTeXcode to construct Figures 6.2 and 6.3

```
\begin{figure}
```

Figure 6.1: A Dendrogram (Tree) Representation for the Ultrametric Component of the Additive Tree Described in the Text Having Vaf of .6359

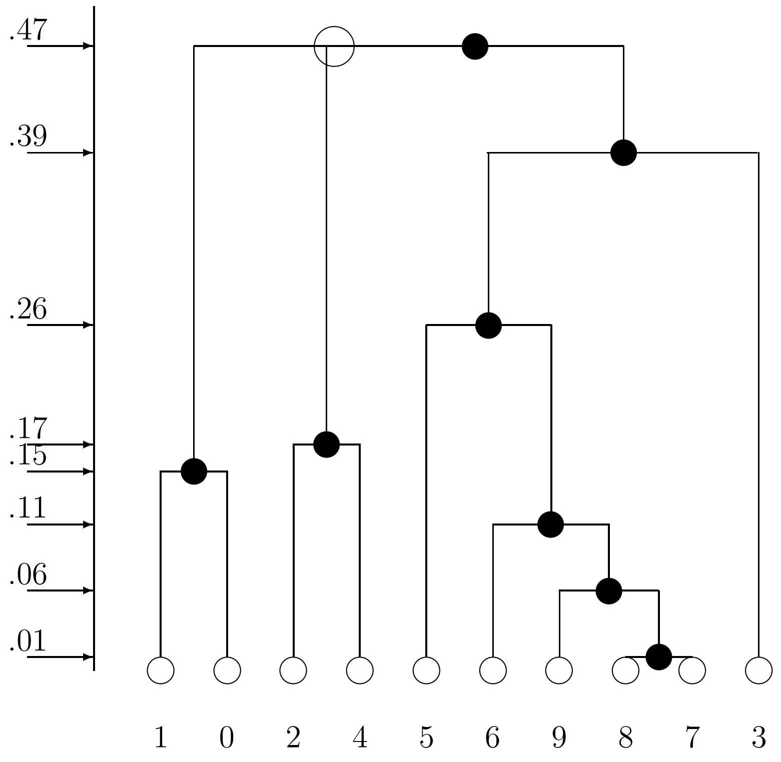
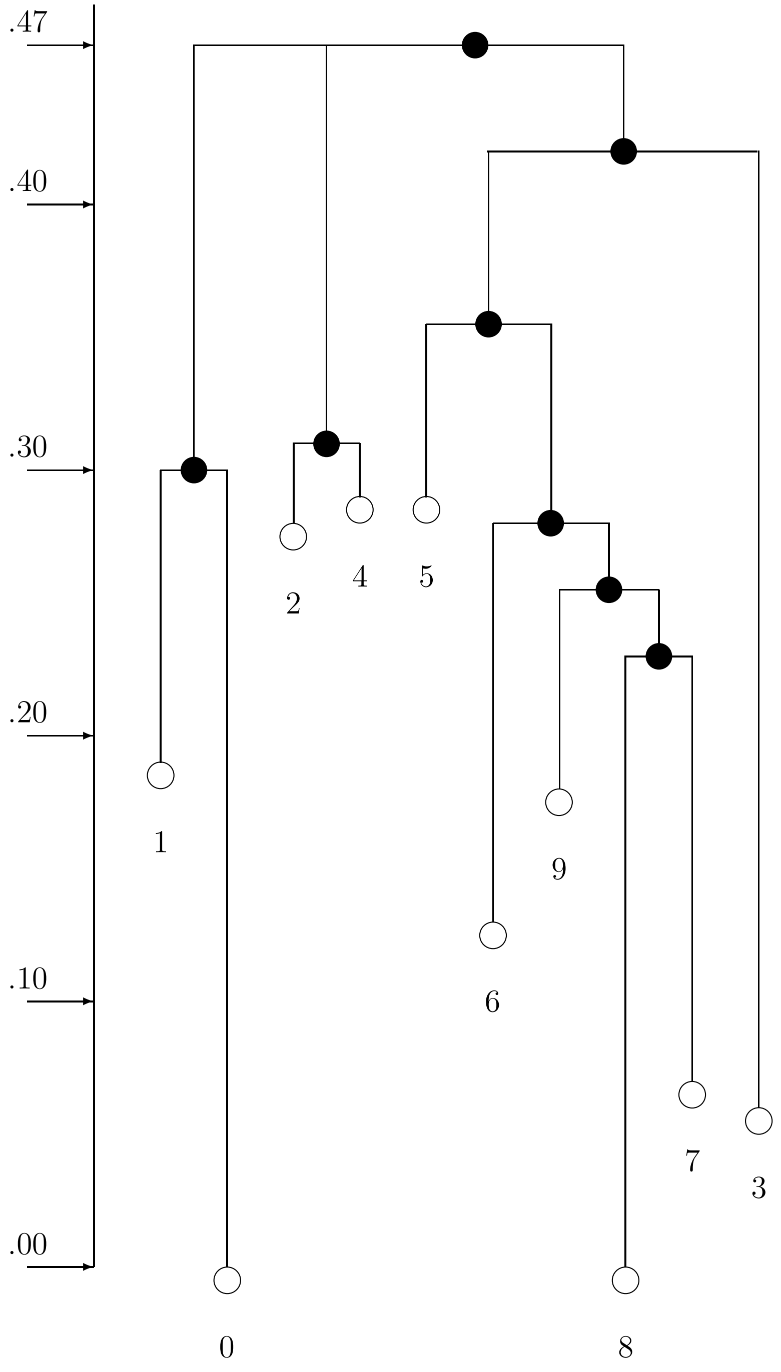


Figure 6.2: A Graph-Theoretic Representation for the Additive Tree Described in the Text Having Vaf of .6359



```
\caption{A Dendrogram (Tree) Representation for the Ultrametric
 Component of the Additive Tree Described in the Text Having Vaf of .6359}

\setlength{\unitlength}{.5pt}

\begin{picture}(500,1000)(0,-250)

\put(50,0){\makebox(0,0){1}}
\put(100,0){\makebox(0,0){0}}
\put(150,0){\makebox(0,0){2}}
\put(200,0){\makebox(0,0){4}}
\put(250,0){\makebox(0,0){5}}
\put(300,0){\makebox(0,0){6}}
\put(350,0){\makebox(0,0){9}}
\put(400,0){\makebox(0,0){8}}
\put(450,0){\makebox(0,0){7}}
\put(500,0){\makebox(0,0){3}}


\put(50,50){\circle{20}}
\put(100,50){\circle{20}}
\put(150,50){\circle{20}}
\put(200,50){\circle{20}}
\put(250,50){\circle{20}}
\put(300,50){\circle{20}}
\put(350,50){\circle{20}}
\put(400,50){\circle{20}}
\put(450,50){\circle{20}}
\put(500,50){\circle{20}}

\put(75,200){\circle*{20}}
\put(175,220){\circle*{20}}
\put(296.875,310){\circle*{20}}
\put(343.75,160){\circle*{20}}
\put(387.5,110){\circle*{20}}
\put(425,60){\circle*{20}}
\put(398.4375,440){\circle*{20}}
\put(286.71875,520){\circle*{20}}
\put(180.859375,520){\circle{30}}

\put(0,50){\line(0,1){500}}
\put(50,60){\line(0,1){140}}
```

```
\put(100,60){\line(0,1){140}}
\put(150,60){\line(0,1){160}}
\put(200,60){\line(0,1){160}}
\put(250,60){\line(0,1){250}}
\put(300,60){\line(0,1){100}}
\put(350,60){\line(0,1){50}}
\put(400,60){\line(0,1){0}}
\put(450,60){\line(0,1){0}}
\put(500,60){\line(0,1){380}}
\put(75,200){\line(0,1){320}}
\put(296.875,310){\line(0,1){130}}
\put(343.75,160){\line(0,1){150}}
\put(175,220){\line(0,1){300}}
\put(398.4375,440){\line(0,1){80}}
\put(286.71875,520){\line(0,1){0}}
\put(425,60){\line(0,1){50}}
\put(387.5,110){\line(0,1){50}}

\put(75,520){\line(1,0){211.71875}}
\put(175,520){\line(1,0){223.4347}}
\put(50,200){\line(1,0){50}}
\put(150,220){\line(1,0){50}}
\put(250,310){\line(1,0){93.75}}
\put(296,440){\line(1,0){203.125}}
\put(400,60){\line(1,0){50}}
\put(350,110){\line(1,0){75}}
\put(300,160){\line(1,0){87.5}}

\put(-50,60){\vector(1,0){50}}
\put(-50,65){\makebox(0,0)[b]{.01}}
\put(-50,110){\vector(1,0){50}}
\put(-50,115){\makebox(0,0)[b]{.06}}
\put(-50,160){\vector(1,0){50}}
\put(-50,165){\makebox(0,0)[b]{.11}}
\put(-50,200){\vector(1,0){50}}
\put(-50,205){\makebox(0,0)[b]{.15}}
\put(-50,220){\vector(1,0){50}}
\put(-50,225){\makebox(0,0)[b]{.17}}
\put(-50,310){\vector(1,0){50}}
\put(-50,315){\makebox(0,0)[b]{.26}}
\put(-50,440){\vector(1,0){50}}
\put(-50,445){\makebox(0,0)[b]{.39}}
```

```
\put(-50,520){\vector(1,0){50}}
\put(-50,525){\makebox(0,0)[b]{.47}}
\end{picture}
\end{figure}



\begin{figure}

\caption{A Graph-Theoretic Representation for the Additive
Tree Described in the Text Having Vaf of .6359}

\setlength{\unitlength}{.5pt}

\begin{picture}(500,1000)(0,-400)

\put(50,-80){\makebox(0,0){1}}
\put(100,-460){\makebox(0,0){0}}
\put(150,100){\makebox(0,0){2}}
\put(200,120){\makebox(0,0){4}}
\put(250,120){\makebox(0,0){5}}
\put(300,-200){\makebox(0,0){6}}
\put(350,-100){\makebox(0,0){9}}
\put(400,-460){\makebox(0,0){8}}
\put(450,-320){\makebox(0,0){7}}
\put(500,-340){\makebox(0,0){3}}


\put(50,-30){\circle{20}}
\put(100,-410){\circle{20}}
\put(150,150){\circle{20}}
\put(200,170){\circle{20}}
\put(250,170){\circle{20}}
\put(300,-150){\circle{20}}
\put(350,-50){\circle{20}}
\put(400,-410){\circle{20}}
\put(450,-270){\circle{20}}
\put(500,-290){\circle{20}}

\put(75,200){\circle*{20}}
\put(175,220){\circle*{20}}
\put(296.875,310){\circle*{20}}
```

```
\put(343.75,160){\circle*{20}}
\put(387.5,110){\circle*{20}}
\put(425,60){\circle*{20}}
\put(398.4375,440){\circle*{20}}
\put(286.71875,520){\circle*{20}}

\put(0,-400){\line(0,1){950}}
\put(50,-20){\line(0,1){220}}
\put(100,-400){\line(0,1){600}}
\put(150,160){\line(0,1){60}}
\put(200,180){\line(0,1){40}}
\put(250,180){\line(0,1){130}}
\put(300,-140){\line(0,1){300}}
\put(350,-40){\line(0,1){150}}
\put(400,-400){\line(0,1){460}}
\put(450,-260){\line(0,1){320}}
\put(500,-280){\line(0,1){720}}
\put(75,200){\line(0,1){320}}
\put(296.875,310){\line(0,1){130}}
\put(343.75,160){\line(0,1){150}}
\put(175,220){\line(0,1){300}}
\put(398.4375,440){\line(0,1){80}}
\put(286.71875,520){\line(0,1){0}}
\put(425,60){\line(0,1){50}}
\put(387.5,110){\line(0,1){50}}

\put(75,520){\line(1,0){211.71875}}
\put(175,520){\line(1,0){223.4347}}
\put(50,200){\line(1,0){50}}
\put(150,220){\line(1,0){50}}
\put(250,310){\line(1,0){93.75}}
\put(296,440){\line(1,0){203.125}}
\put(400,60){\line(1,0){50}}
\put(350,110){\line(1,0){75}}
\put(300,160){\line(1,0){87.5}}

\put(-50,-400){\vector(1,0){50}}
\put(-50,-390){\makebox(0,0)[b]{.00}}
\put(-50,-200){\vector(1,0){50}}
\put(-50,-190){\makebox(0,0)[b]{.10}}
\put(-50,0){\vector(1,0){50}}
\put(-50,10){\makebox(0,0)[b]{.20}}
```

```
\put(-50,200){\vector(1,0){50}}
\put(-50,210){\makebox(0,0)[b]{.30}}
\put(-50,400){\vector(1,0){50}}
\put(-50,410){\makebox(0,0)[b]{.40}}
\put(-50,520){\vector(1,0){50}}
\put(-50,530){\makebox(0,0)[b]{.47}}

\end{picture}
\end{figure}
```

6.5 An Alternative for Finding an Additive Tree in the L_2 Norm (Based on Combining a Centroid Metric and an Ultrametric)

If the four-point condition characterizing an additive tree is strengthened so that all the sums in the defining conditions for all object quadruples are equal (and not only for the largest two such sums), the additive tree matrix so obtained has entries representable as $g_i + g_j$, for a collection of values $g_1, \ldots, g_n$. This specially constrained additive tree is usually referred to as a centroid metric, and as noted by Carroll and Pruzansky (1980) and De Soete, DeSarbo, Furnas, and Carroll (1984), can be fitted to a proximity matrix in the L_2-norm through closed-form expressions. Specifically, if $\mathbf{P}$ denotes the proximity matrix, then g_i can be given as the i^{th} row sum of $\mathbf{P}$ excluding the diagonal entry, divided by $n-2$, minus the total off-diagonal sum divided by $2(n-1)(n-2)$.

The m-file, `centfit.m`, for obtaining the best-fitting centroid metric in the L_2-norm, has usage

```
function [fit,vaf,lengths] = centfit(prox)
```

where `PROX` is the usual input proximity matrix (with a zero main diagonal and a dissimilarity interpretation); the n values that serve to define the approximating sums, $g_i + g_j$, present in the fitted matrix `FIT`, are given in the vector `LENGTHS` of size $n \times 1$. The example below uses `centfit.m` with the `number.dat` data set, leading to an additive tree with vaf of .3248; the latter could be represented graphically as a "star" tree with one internal node and spokes having the lengths given in the output vector `LENGTHS`

```
load number.dat
[fit,vaf,lengths] = centfit(number)

fit =

  Columns 1 through 7
```

```
         0    0.7808    0.6877    0.6709    0.6784    0.7647    0.6589
    0.7808         0    0.5026    0.4858    0.4933    0.5796    0.4738
    0.6877    0.5026         0    0.3927    0.4002    0.4864    0.3807
    0.6709    0.4858    0.3927         0    0.3834    0.4697    0.3639
    0.6784    0.4933    0.4002    0.3834         0    0.4772    0.3714
    0.7647    0.5796    0.4864    0.4697    0.4772         0    0.4577
    0.6589    0.4738    0.3807    0.3639    0.3714    0.4577         0
    0.8128    0.6277    0.5346    0.5178    0.5253    0.6116    0.5058
    0.7499    0.5648    0.4717    0.4549    0.4624    0.5487    0.4429
    0.7657    0.5806    0.4874    0.4707    0.4782    0.5644    0.4587

  Columns 8 through 10

    0.8128    0.7499    0.7657
    0.6277    0.5648    0.5806
    0.5346    0.4717    0.4874
    0.5178    0.4549    0.4707
    0.5253    0.4624    0.4782
    0.6116    0.5487    0.5644
    0.5058    0.4429    0.4587
         0    0.5968    0.6126
    0.5968         0    0.5497
    0.6126    0.5497         0

vaf =

    0.3248

lengths =

  Columns 1 through 7

    0.4830    0.2978    0.2047    0.1880    0.1955    0.2817    0.1760

  Columns 8 through 10

    0.3298    0.2670    0.2827
```

An alternative strategy for identifying good-fitting additive trees (and one that will be used in a slightly different form on two-mode proximity data in Section 8.2) relies on the possible decomposition of an additive tree into an ultrametric and centroid metric. The m-file, `atreectul.m`, first fits a centroid metric in closed form; an ultrametric is then identified on the residual matrix. The sum of these two matrices is an additive tree. The usage would follow that of `atreefnd.m`:

```
[find,vaf] = atreectul(prox,inperm)
```

where `FIND` is the identified additive tree with variance-accounted-for `VAF`. Again, the matrix `PROX` contains the symmetric input proximities, and `INPERM` is a permutation that defines an order in which the constraints are considered over all object triples in the identification of the ultrametric component. In the example below, one search is shown starting with a random permutation (through the use of `randperm(10)`) that gives the same additive tree identified earlier with a vaf of .6249.

```
[find,vaf] = atreectul(number,randperm(10))

find =

  Columns 1 through 7

        0    0.4210    0.7185    0.7371    0.7092    0.8188    0.7116
   0.4210         0    0.5334    0.5520    0.5241    0.6337    0.5265
   0.7185    0.5334         0    0.4882    0.0590    0.5700    0.4627
   0.7371    0.5520    0.4882         0    0.4790    0.4337    0.2506
   0.7092    0.5241    0.0590    0.4790         0    0.5607    0.4535
   0.8188    0.6337    0.5700    0.4337    0.5607         0    0.4082
   0.7116    0.5265    0.4627    0.2506    0.4535    0.4082         0
   0.8670    0.6818    0.6181    0.4818    0.6089    0.4000    0.4563
   0.7549    0.5698    0.3111    0.5247    0.3019    0.6064    0.4992
   0.8318    0.6467    0.5830    0.2630    0.5737    0.5284    0.3454

  Columns 8 through 10

   0.8670    0.7549    0.8318
   0.6818    0.5698    0.6467
   0.6181    0.3111    0.5830
   0.4818    0.5247    0.2630
   0.6089    0.3019    0.5737
   0.4000    0.6064    0.5284
   0.4563    0.4992    0.3454
        0    0.6546    0.5766
   0.6546         0    0.6194
   0.5766    0.6194         0
```

```
vaf =

    0.6249
```

Chapter 7

Fitting Multiple Tree Structures to a Symmetric Proximity Matrix

The use of multiple structures, whether they be ultrametrics or additive trees, to additively represent a given proximity matrix, proceeds directly through successive residualization and iteration. We restrict ourselves to the fitting of two such structures but the same process would apply for any such number. Initially, a first matrix is fitted to a given proximity matrix and a first residual matrix obtained; a second structure is then fitted to these first residuals, producing a second residual matrix. Iterating, the second fitted matrix is now subtracted from the original proximity matrix and a first (re)fitted matrix obtained; this first (re)fitted matrix in turn is subtracted from the original proximity matrix and a new second matrix (re)fitted. This process continues until the variance-accounted-for by the sum of both fitted matrices no longer changes by a set amount (the value of 1.0e-006 is used in the m-files of the next two sections).

7.1 Multiple Ultrametrics

The m-file, `biultrafnd`, fits (additively) two ultrametric matrices in the L_2-norm. The explicit usage is

```
[find,vaf,targone,targtwo] = biultrafnd(prox,inperm)
```

where `PROX` is the given input proximity matrix (with a zero main diagonal and a dissimilarity interpretation); `INPERM` is a permutation that determines the order in which the inequality constraints are considered (and thus can be made random to search for different locally optimal representations); `FIND` is the found least-squares matrix (with variance-accounted-for of `VAF`) to `PROX`, and is the sum of the two ultrametric matrices `TARGONE` and `TARGTWO`.

In the example to follow, a vaf of .8001 was achieved for the two identified ultrametrics (and where one needs to add an (arbitrary) constant [e.g., of .40] to the entries in `TARGTWO` to satisfy the technical requirement that ultrametric values should be nonnegative). It might be noted substantively that the first ultrametric matrix (in `TARGONE`) reflects the structural properties of the digits; the second ultrametric matrix (in `TARGTWO`) is completely consistent with digit magnitude. This is a very nice mixture of ultrametric structures with a convenient substantive interpretation for both components.

```
[find,vaf,targone,targtwo] = biultrafnd(number,randperm(10))

find =

  Columns 1 through 7

         0    0.4210    0.5266    0.6075    0.7685    0.7685    0.8694
    0.4210         0    0.3414    0.4224    0.5834    0.5834    0.6843
    0.5266    0.3414         0    0.3791    0.0589    0.5401    0.6410
    0.6075    0.4224    0.3791         0    0.5401    0.4511    0.3669
    0.7685    0.5834    0.0589    0.5401         0    0.4090    0.6410
    0.7685    0.5834    0.5401    0.4511    0.4090         0    0.5519
    0.8694    0.6843    0.6410    0.3669    0.6410    0.5519         0
    0.8694    0.6843    0.6410    0.5519    0.6410    0.4000    0.3640
    0.8694    0.6843    0.3065    0.6410    0.3065    0.6410    0.3500
    0.8694    0.6843    0.6410    0.2630    0.6410    0.5519    0.2293

  Columns 8 through 10

    0.8694    0.8694    0.8694
    0.6843    0.6843    0.6843
    0.6410    0.3065    0.6410
    0.5519    0.6410    0.2630
    0.6410    0.3065    0.6410
    0.4000    0.6410    0.5519
    0.3640    0.3500    0.2293
         0    0.4530    0.4143
    0.4530         0    0.5034
    0.4143    0.5034         0


vaf =

    0.8001


targone =

  Columns 1 through 7
```

```
         0    0.7796    0.7796    0.7796    0.7796    0.7796    0.7796
    0.7796         0    0.5945    0.5945    0.5945    0.5945    0.5945
    0.7796    0.5945         0    0.5512    0.0701    0.5512    0.5512
    0.7796    0.5945    0.5512         0    0.5512    0.4622    0.2772
    0.7796    0.5945    0.0701    0.5512         0    0.5512    0.5512
    0.7796    0.5945    0.5512    0.4622    0.5512         0    0.4622
    0.7796    0.5945    0.5512    0.2772    0.5512    0.4622         0
    0.7796    0.5945    0.5512    0.4622    0.5512    0.3103    0.4622
    0.7796    0.5945    0.2168    0.5512    0.2168    0.5512    0.5512
    0.7796    0.5945    0.5512    0.1733    0.5512    0.4622    0.2772

  Columns 8 through 10

    0.7796    0.7796    0.7796
    0.5945    0.5945    0.5945
    0.5512    0.2168    0.5512
    0.4622    0.5512    0.1733
    0.5512    0.2168    0.5512
    0.3103    0.5512    0.4622
    0.4622    0.5512    0.2772
         0    0.5512    0.4622
    0.5512         0    0.5512
    0.4622    0.5512         0


targtwo =

  Columns 1 through 7

         0   -0.3586   -0.2531   -0.1721   -0.0111   -0.0111    0.0897
   -0.3586         0   -0.2531   -0.1721   -0.0111   -0.0111    0.0897
   -0.2531   -0.2531         0   -0.1721   -0.0111   -0.0111    0.0897
   -0.1721   -0.1721   -0.1721         0   -0.0111   -0.0111    0.0897
   -0.0111   -0.0111   -0.0111   -0.0111         0   -0.1422    0.0897
   -0.0111   -0.0111   -0.0111   -0.0111   -0.1422         0    0.0897
    0.0897    0.0897    0.0897    0.0897    0.0897    0.0897         0
    0.0897    0.0897    0.0897    0.0897    0.0897    0.0897   -0.0982
    0.0897    0.0897    0.0897    0.0897    0.0897    0.0897   -0.2012
    0.0897    0.0897    0.0897    0.0897    0.0897    0.0897   -0.0479

  Columns 8 through 10
```

```
    0.0897    0.0897    0.0897
    0.0897    0.0897    0.0897
    0.0897    0.0897    0.0897
    0.0897    0.0897    0.0897
    0.0897    0.0897    0.0897
    0.0897    0.0897    0.0897
   -0.0982   -0.2012   -0.0479
         0   -0.0982   -0.0479
   -0.0982         0   -0.0479
   -0.0479   -0.0479         0

[orderprox,orderperm] = ultraorder(targone)

orderprox =

  Columns 1 through 7

         0    0.7796    0.7796    0.7796    0.7796    0.7796    0.7796
    0.7796         0    0.2168    0.2168    0.5512    0.5512    0.5512
    0.7796    0.2168         0    0.0701    0.5512    0.5512    0.5512
    0.7796    0.2168    0.0701         0    0.5512    0.5512    0.5512
    0.7796    0.5512    0.5512    0.5512         0    0.1733    0.2772
    0.7796    0.5512    0.5512    0.5512    0.1733         0    0.2772
    0.7796    0.5512    0.5512    0.5512    0.2772    0.2772         0
    0.7796    0.5512    0.5512    0.5512    0.4622    0.4622    0.4622
    0.7796    0.5512    0.5512    0.5512    0.4622    0.4622    0.4622
    0.7796    0.5945    0.5945    0.5945    0.5945    0.5945    0.5945

  Columns 8 through 10

    0.7796    0.7796    0.7796
    0.5512    0.5512    0.5945
    0.5512    0.5512    0.5945
    0.5512    0.5512    0.5945
    0.4622    0.4622    0.5945
    0.4622    0.4622    0.5945
    0.4622    0.4622    0.5945
         0    0.3103    0.5945
    0.3103         0    0.5945
    0.5945    0.5945         0
```

```
orderperm =

     1     9     3     5    10     4     7     8     6     2

[orderprox,orderperm] = ultraorder(targtwo)

orderprox =

  Columns 1 through 7

         0   -0.3586   -0.2531   -0.1721   -0.0111   -0.0111    0.0897
   -0.3586         0   -0.2531   -0.1721   -0.0111   -0.0111    0.0897
   -0.2531   -0.2531         0   -0.1721   -0.0111   -0.0111    0.0897
   -0.1721   -0.1721   -0.1721         0   -0.0111   -0.0111    0.0897
   -0.0111   -0.0111   -0.0111   -0.0111         0   -0.1422    0.0897
   -0.0111   -0.0111   -0.0111   -0.0111   -0.1422         0    0.0897
    0.0897    0.0897    0.0897    0.0897    0.0897    0.0897         0
    0.0897    0.0897    0.0897    0.0897    0.0897    0.0897   -0.0982
    0.0897    0.0897    0.0897    0.0897    0.0897    0.0897   -0.0982
    0.0897    0.0897    0.0897    0.0897    0.0897    0.0897   -0.0479

  Columns 8 through 10

    0.0897    0.0897    0.0897
    0.0897    0.0897    0.0897
    0.0897    0.0897    0.0897
    0.0897    0.0897    0.0897
    0.0897    0.0897    0.0897
    0.0897    0.0897    0.0897
   -0.0982   -0.0982   -0.0479
         0   -0.2012   -0.0479
   -0.2012         0   -0.0479
   -0.0479   -0.0479         0


orderperm =

     1     2     3     4     5     6     8     7     9    10
```

7.2 Multiple Additive Trees

The m-file, `biatreefnd`, fits (additively) two additive tree matrices in the L_2-norm. The explicit usage is

```
[find,vaf,targone,targtwo] = biatreefnd(prox,inperm)
```

where `PROX` is the given input proximity matrix (with a zero main diagonal and a dissimilarity interpretation); `INPERM` is a permutation that determines the order in which the inequality constraints are considered (and thus can be made random to search for different locally optimal representations); `FIND` is the found least-squares matrix (with variance-accounted-for of `VAF`) to `PROX`, and is the sum of the two additive tree matrices `TARGONE` and `TARGTWO`.

In the example to follow, a vaf of .9003 was achieved for the two identified additive trees (and where one needs as in the multiple ultrametric case, to add an (arbitrary) constant [e.g., of .40] to the entries in `TARGTWO` to satisfy the technical requirement that additive tree values should be nonnegative). Similarly, as in the interpretation for the example of the last section, it might be noted substantively that the second additive tree matrix (in `TARGTWO`) reflects the structural properties of the digits; the first matrix (in `TARGONE`) is completely consistent with digit magnitude. So, again we have a very nice mixture of structures with convenient substantive interpretations for both components.

```
load number.dat
[find,vaf,targone,targtwo] = biatreefnd(number,randperm(10))
find =

  Columns 1 through 7

         0    0.4210    0.4955    0.6196    0.7487    0.7882    0.7083
    0.4210         0    0.3725    0.3411    0.6256    0.5723    0.5852
    0.4955    0.3725         0    0.4483    0.0590    0.6169    0.4747
    0.6196    0.3411    0.4483         0    0.4683    0.4150    0.4279
    0.7487    0.6256    0.0590    0.4683         0    0.4090    0.3766
    0.7882    0.5723    0.6169    0.4150    0.4090         0    0.4784
    0.7083    0.5852    0.4747    0.4279    0.3766    0.4784         0
    0.9558    0.7399    0.7845    0.5826    0.6864    0.4000    0.4013
    0.9246    0.8015    0.3556    0.6442    0.2574    0.6947    0.3078
    0.9084    0.6299    0.7371    0.2630    0.6390    0.5857    0.3539

  Columns 8 through 10

    0.9558    0.9246    0.9084
    0.7399    0.8015    0.6299
    0.7845    0.3556    0.7371
    0.5826    0.6442    0.2630
    0.6864    0.2574    0.6390
    0.4000    0.6947    0.5857
    0.4013    0.3078    0.3539
         0    0.4000    0.3947
    0.4000         0    0.4563
    0.3947    0.4563         0


vaf =

    0.9003


targone =

  Columns 1 through 7

         0    0.4439    0.4582    0.6163    0.7114    0.7976    0.7699
    0.4439         0    0.2731    0.4312    0.5262    0.6125    0.5848
    0.4582    0.2731         0    0.3227    0.4178    0.5040    0.4763
    0.6163    0.4312    0.3227         0    0.3427    0.4290    0.4013
    0.7114    0.5262    0.4178    0.3427         0    0.2961    0.3782
    0.7976    0.6125    0.5040    0.4290    0.2961         0    0.4644
    0.7699    0.5848    0.4763    0.4013    0.3782    0.4644         0
    0.9652    0.7801    0.6716    0.5966    0.5735    0.6598    0.3874
    0.9023    0.7172    0.6087    0.5337    0.5106    0.5969    0.3245
    0.9051    0.7200    0.6115    0.5365    0.5134    0.5997    0.3273

  Columns 8 through 10

    0.9652    0.9023    0.9051
    0.7801    0.7172    0.7200
    0.6716    0.6087    0.6115
    0.5966    0.5337    0.5365
    0.5735    0.5106    0.5134
    0.6598    0.5969    0.5997
    0.3874    0.3245    0.3273
         0    0.3022    0.4087
    0.3022         0    0.3458
    0.4087    0.3458         0
```

```
targtwo =

  Columns 1 through 7

         0   -0.0229    0.0373    0.0033    0.0373   -0.0094   -0.0616
   -0.0229         0    0.0994   -0.0901    0.0994   -0.0402    0.0005
    0.0373    0.0994         0    0.1256   -0.3588    0.1129   -0.0016
    0.0033   -0.0901    0.1256         0    0.1256   -0.0140    0.0267
    0.0373    0.0994   -0.3588    0.1256         0    0.1129   -0.0016
   -0.0094   -0.0402    0.1129   -0.0140    0.1129         0    0.0139
   -0.0616    0.0005   -0.0016    0.0267   -0.0016    0.0139         0
   -0.0094   -0.0402    0.1129   -0.0140    0.1129   -0.2598    0.0139
    0.0222    0.0843   -0.2532    0.1105   -0.2532    0.0978   -0.0167
    0.0033   -0.0901    0.1256   -0.2735    0.1256   -0.0140    0.0267

  Columns 8 through 10

   -0.0094    0.0222    0.0033
   -0.0402    0.0843   -0.0901
    0.1129   -0.2532    0.1256
   -0.0140    0.1105   -0.2735
    0.1129   -0.2532    0.1256
   -0.2598    0.0978   -0.0140
    0.0139   -0.0167    0.0267
         0    0.0978   -0.0140
    0.0978         0    0.1105
   -0.0140    0.1105         0

[ulmetricone,ctmetricone] = atreedec(targone,0.0)

ulmetricone =

  Columns 1 through 7

         0   -1.3014   -1.1786   -0.9652   -0.9652   -0.9652   -0.9652
   -1.3014         0   -1.1786   -0.9652   -0.9652   -0.9652   -0.9652
   -1.1786   -1.1786         0   -0.9652   -0.9652   -0.9652   -0.9652
   -0.9652   -0.9652   -0.9652         0   -0.9850   -0.9850   -0.9850
   -0.9652   -0.9652   -0.9652   -0.9850         0   -1.2128   -1.1031
   -0.9652   -0.9652   -0.9652   -0.9850   -1.2128         0   -1.1031
   -0.9652   -0.9652   -0.9652   -0.9850   -1.1031   -1.1031         0
   -0.9652   -0.9652   -0.9652   -0.9850   -1.1031   -1.1031   -1.3477
   -0.9652   -0.9652   -0.9652   -0.9850   -1.1031   -1.1031   -1.3477
   -0.9652   -0.9652   -0.9652   -0.9850   -1.1031   -1.1031   -1.3477

  Columns 8 through 10

   -0.9652   -0.9652   -0.9652
   -0.9652   -0.9652   -0.9652
   -0.9652   -0.9652   -0.9652
   -0.9850   -0.9850   -0.9850
   -1.1031   -1.1031   -1.1031
   -1.1031   -1.1031   -1.1031
   -1.3477   -1.3477   -1.3477
         0   -1.5653   -1.4617
   -1.5653         0   -1.4617
   -1.4617   -1.4617         0


ctmetricone =

    0.9652
    0.7801
    0.6716
    0.6163
    0.7114
    0.7976
    0.7699
    0.9652
    0.9023
    0.9051

[ulmetrictwo,ctmetrictwo] = atreedec(targtwo,0.0)

ulmetrictwo =

  Columns 1 through 7

         0   -0.1596   -0.1256   -0.1596   -0.1256   -0.1596   -0.1256
   -0.1596         0   -0.1256   -0.3151   -0.1256   -0.2525   -0.1256
   -0.1256   -0.1256         0   -0.1256   -0.6099   -0.1256   -0.1539
   -0.1596   -0.3151   -0.1256         0   -0.1256   -0.2525   -0.1256
   -0.1256   -0.1256   -0.6099   -0.1256         0   -0.1256   -0.1539
   -0.1596   -0.2525   -0.1256   -0.2525   -0.1256         0   -0.1256
   -0.1256   -0.1256   -0.1539   -0.1256   -0.1539   -0.1256         0
   -0.1596   -0.2525   -0.1256   -0.2525   -0.1256   -0.4855   -0.1256
   -0.1256   -0.1256   -0.4893   -0.1256   -0.4893   -0.1256   -0.1539
   -0.1596   -0.3151   -0.1256   -0.5247   -0.1256   -0.2525   -0.1256

  Columns 8 through 10

   -0.1596   -0.1256   -0.1596
   -0.2525   -0.1256   -0.3151
   -0.1256   -0.4893   -0.1256
   -0.2525   -0.1256   -0.5247
   -0.1256   -0.4893   -0.1256
   -0.4855   -0.1256   -0.2525
   -0.1256   -0.1539   -0.1256
         0   -0.1256   -0.2525
   -0.1256         0   -0.1256
   -0.2525   -0.1256         0


ctmetrictwo =

    0.0373
    0.0994
    0.1256
    0.1256
    0.1256
    0.1129
    0.0267
    0.1129
    0.1105
    0.1256

[orderproxone,orderpermone] = ultraorder(ulmetricone)

orderproxone =

  Columns 1 through 7

         0   -1.1786   -1.1786   -0.9652   -0.9652   -0.9652   -0.9652
   -1.1786         0   -1.3014   -0.9652   -0.9652   -0.9652   -0.9652
   -1.1786   -1.3014         0   -0.9652   -0.9652   -0.9652   -0.9652
   -0.9652   -0.9652   -0.9652         0   -1.2128   -1.1031   -1.1031
   -0.9652   -0.9652   -0.9652   -1.2128         0   -1.1031   -1.1031
   -0.9652   -0.9652   -0.9652   -1.1031   -1.1031         0   -1.4617
   -0.9652   -0.9652   -0.9652   -1.1031   -1.1031   -1.4617         0
   -0.9652   -0.9652   -0.9652   -1.1031   -1.1031   -1.4617   -1.5653
   -0.9652   -0.9652   -0.9652   -1.1031   -1.1031   -1.3477   -1.3477
   -0.9652   -0.9652   -0.9652   -0.9850   -0.9850   -0.9850   -0.9850

  Columns 8 through 10

   -0.9652   -0.9652   -0.9652
   -0.9652   -0.9652   -0.9652
   -0.9652   -0.9652   -0.9652
   -1.1031   -1.1031   -0.9850
   -1.1031   -1.1031   -0.9850
   -1.4617   -1.3477   -0.9850
   -1.5653   -1.3477   -0.9850
         0   -1.3477   -0.9850
   -1.3477         0   -0.9850
   -0.9850   -0.9850         0


orderpermone =

     3     2     1     5     6    10     9     8     7     4

[orderproxtwo,orderpermtwo] = ultraorder(ulmetrictwo)

orderproxtwo =

  Columns 1 through 7

         0   -0.1539   -0.1539   -0.1539   -0.1256   -0.1256   -0.1256
   -0.1539         0   -0.4893   -0.4893   -0.1256   -0.1256   -0.1256
   -0.1539   -0.4893         0   -0.6099   -0.1256   -0.1256   -0.1256
   -0.1539   -0.4893   -0.6099         0   -0.1256   -0.1256   -0.1256
   -0.1256   -0.1256   -0.1256   -0.1256         0   -0.5247   -0.3151
   -0.1256   -0.1256   -0.1256   -0.1256   -0.5247         0   -0.3151
   -0.1256   -0.1256   -0.1256   -0.1256   -0.3151   -0.3151         0
   -0.1256   -0.1256   -0.1256   -0.1256   -0.2525   -0.2525   -0.2525
   -0.1256   -0.1256   -0.1256   -0.1256   -0.2525   -0.2525   -0.2525
   -0.1256   -0.1256   -0.1256   -0.1256   -0.1596   -0.1596   -0.1596
  Columns 8 through 10

   -0.1256   -0.1256   -0.1256
   -0.1256   -0.1256   -0.1256
   -0.1256   -0.1256   -0.1256
   -0.1256   -0.1256   -0.1256
   -0.2525   -0.2525   -0.1596
   -0.2525   -0.2525   -0.1596
   -0.2525   -0.2525   -0.1596
         0   -0.4855   -0.1596
   -0.4855         0   -0.1596
   -0.1596   -0.1596         0


orderpermtwo =

     7     9     5     3    10     4     2     8     6     1
```

Chapter 8

Ultrametrics and Additive Trees for Two-Mode (Rectangular) Proximity Data

The proximity data considered thus far for obtaining some type of structural representation, such as an ultrametric or an additive tree, have been assumed to be on one intact set of objects, $S = \{O_1, \ldots, O_n\}$, and complete in the sense that proximity values are present between all object pairs. Suppose now that the available proximity data are two-mode, that is *between* two distinct object sets, $S_A = \{O_{1A}, \ldots, O_{n_aA}\}$ and $S_B = \{O_{1B}, \ldots, O_{n_bB}\}$, containing n_a and n_b objects, respectively, and defined through an $n_a \times n_b$ proximity matrix $\mathbf{Q} = \{q_{rs}\}$, where again, for convenience, we assume that the entries in $\mathbf{Q}$ are keyed as dissimilarities. What may be desirable is a joint structural representation of the set $S_A \cup S_B$ (considered as a single object set S containing $n_a + n_b = n$ objects), but one that is based only on the available proximities between the sets S_A and S_B.

Conditions have been proposed in the literature for when the entries in a matrix fitted to $\mathbf{Q}$ characterize an ultrametric or an additive tree representation. In particular, suppose a $n_a \times n_b$ matrix $\mathbf{F} = \{f_{rs}\}$ is fitted to $\mathbf{Q}$ through least squares subject to the constraints that follow:

Ultrametric (Furnas, 1980):

for all distinct object quadruples, O_{rA}, O_{sA}, O_{rB}, O_{sB}, where O_{rA}, $O_{sA} \in S_A$ and O_{rB}, O_{sB}, $\in S_B$, and considering the entries in $\mathbf{F}$ corresponding to the pairs, (O_{rA}, O_{rB}), (O_{rA}, O_{sB}), (O_{sA} O_{rB}), and (O_{sA}, O_{sB}), say $f_{r_Ar_B}$, $f_{r_As_B}$, $f_{s_Ar_B}$, $f_{s_As_B}$, respectively, the largest two must be equal.

Additive trees (Brossier, 1987):

for all distinct object sextuples, O_{rA}, O_{sA}, O_{tA}, O_{rB}, O_{sB}, O_{tB}, where O_{rA}, O_{sA}, $O_{tA} \in S_A$ and O_{rB}, O_{sB}, O_{tB}, $\in S_B$, and considering the entries in $\mathbf{F}$ corresponding to the pairs (O_{rA}, O_{rB}), (O_{rA}, O_{sB}), (O_{rA}, O_{tB}), (O_{sA}, O_{rB}), (O_{sA}, O_{sB}), (O_{sA}, O_{tB}), (O_{tA}, O_{rB}), (O_{tA}, O_{sB}), and (O_{tA}, O_{tB}), say $f_{r_A r_B}$, $f_{r_A s_B}$, $f_{r_A t_B}$, $f_{s_A r_B}$, $f_{s_A s_B}$, $f_{s_A t_B}$, $f_{t_A r_B}$, $f_{t_A s_B}$, $f_{t_A t_B}$, respectively, the largest two of the following sums must be equal:

$f_{r_A r_B} + f_{s_A s_B} + f_{t_A t_B}$;
$f_{r_A r_B} + f_{s_A t_B} + f_{t_A s_B}$;
$f_{r_A s_B} + f_{s_A r_B} + f_{t_A t_B}$;
$f_{r_A s_B} + f_{s_A t_B} + f_{t_A r_B}$;
$f_{r_A t_B} + f_{s_A r_B} + f_{t_A s_B}$;
$f_{r_A t_B} + f_{s_A s_B} + f_{t_A r_B}$.

In both cases of ultrametric and additive trees for two-mode proximity data, the necessary constraints characterizing a solution are linear and define closed convex sets in which a solution must lie. Thus, the application of iterative projection as a heuristic search strategy for the best-fitting solutions is fairly direct, and an example of an ultrametric found and fitted to a two-mode matrix will be given in Section 8.1. We will not, however, give a comparable example of fitting the additive tree constraints to such a proximity matrix; the (scratch) storage requirements necessitated by iterative projection in directly using the additive tree constraints given above and keeping track of the various augmentations made in the course of the heuristic search can become rather onerous for moderate-sized data matrices. For general use, an alternative approach to the fitting of additive trees is preferable that again uses iterative projection but with the ultrametric conditions in conjunction with a secondary centroid metric; this strategy avoids any major (scratch) storage difficulties and will be reviewed and illustrated in Section 8.2.

We might note that the process of fitting two-mode proximity data by additive trees or ultrametrics using iterative projection heuristics may generate a rather large number of distinct locally optimal solutions, particularly in contrast to the situation usually observed for symmetric proximity data. Although this abundance is not inevitably the case and obviously depends on the particular data set being considered, it is not unusual and should be expected by a user.

8.1 Fitting and Finding Two-Mode Ultrametrics

To illustrate the fitting of a given two-mode ultrametric, a two-mode target is generated by the upper-right 6×4 portion of the 10×10 ultrametric target matrix, `numcltarg`, used in Section 5.1. This file will be called `numcltarg6x4.dat`, and has contents as follows:

```
9 9 9 9
9 9 9 9
8 8 4 8
3 7 8 2
8 8 4 8
7 5 8 7
```

The six rows correspond to the digits 0, 1, 2, 3, 4, and 5; the four columns to 6, 7, 8, and 9. As the two-mode 6×4 proximity matrix, the appropriate upper-right portion of the `number` proximity matrix will be used in the fitting process; the corresponding file is called `number6x4.dat`, with contents:

```
.788 .909 .821 .850
.758 .630 .791 .625
.421 .796 .367 .808
.300 .592 .804 .263
.388 .742 .246 .683
.396 .400 .671 .592
```

The m-file, `ultrafittm.m`, fits a given ultrametric to a two-mode proximity matrix (using iterative projection in the L_2-norm); it has usage

```
[fit,vaf] = ultrafittm(proxtm,targ)
```

where `PROXTM` is the two-mode (rectangular) input proximity matrix (with a dissimilarity interpretation); `TARG` is an ultrametric matrix of the same size as `PROXTM`; `FIT` is the least-squares optimal matrix (with variance-accounted-for of `VAF`) to `PROXTM` satisfying the two-mode ultrametric constraints implicit in `TARG`. An example follows using `numcltarg6x4` for `TARG` and `number6x4` as `PROXTM`:

```
load number6x4.dat
number6x4

number6x4 =

    0.7880    0.9090    0.8210    0.8500
    0.7580    0.6300    0.7910    0.6250
    0.4210    0.7960    0.3670    0.8080
    0.3000    0.5920    0.8040    0.2630
    0.3880    0.7420    0.2460    0.6830
    0.3960    0.4000    0.6710    0.5920

load numcltarg6x4.dat
numcltarg6x4

numcltarg6x4 =

     9     9     9     9
     9     9     9     9
     8     8     4     8
     3     7     8     2
     8     8     4     8
     7     5     8     7


[fit,vaf] = ultrafittm(number6x4,numcltarg6x4)

fit =

    0.7715    0.7715    0.7715    0.7715
    0.7715    0.7715    0.7715    0.7715
    0.6641    0.6641    0.3065    0.6641
    0.3000    0.5267    0.6641    0.2630
    0.6641    0.6641    0.3065    0.6641
    0.5267    0.4000    0.6641    0.5267


vaf =

    0.6978
```

A vaf of .6978 was obtained for the fitted ultrametric; we give the hierarchy below with indications of when the partitions were formed in the L_2-norm fitted ultrametric (in `FIT`) and in the original target (in `cltarg6X4`):

Partition	Level Formed (L_2)	Level Formed (Target)
{{0,1,2,4,8,3,9,6,5,7}}	.7715	9
{{0},{1},{2,4,8,3,9,6,5,7}}	.6641	8
{{0},{1},{2,4,8},{3,9,6,5,7}}	.5267	7
{{0},{1},{2,4,8},{3,9,6},{5,7}}	.4000	5
{{0},{1},{2,4,8},{3,9,6},{5},{7}}	.3065	4
{{0},{1},{2},{4},{8},{3,9,6},{5},{7}}	.3000	3
{{0},{1},{2},{4},{8},{3,9},{6},{5},{7}}	.2630	2
{{0},{1},{2},{4},{8},{3},{9},{6},{5},{7}}	—	—

The m-file, `ultrafndtm.m`, relies on iterative projection heuristically to locate a best-fitting two-mode ultrametric. The usage is

```
[find,vaf] = ultrafndtm(proxtm,inpermrow,inpermcol)
```

where `PROXTM` is the two-mode input proximity matrix (with a dissimilarity interpretation); `INPERMROW` and `INPERMCOL` are permutations for the row and column objects that determine the order in which the inequality constraints are considered; `FIND` is the found least-squares matrix (with variance-accounted-for of `VAF`) to `PROXTM` satisfying the ultrametric constraints. The example below for the `number6x4` two-mode data (using random permutations for `INPERMROW` and `INPERMCOL`), finds an ultrametric with vaf of .7448.

```
[find,vaf] = ultrafndtm(number6x4,randperm(6),randperm(4))

find =

    0.8420    0.8420    0.8420    0.8420
    0.7010    0.7010    0.7010    0.7010
    0.6641    0.6641    0.3670    0.6641
    0.3000    0.5267    0.6641    0.2630
    0.6641    0.6641    0.2460    0.6641
    0.5267    0.4000    0.6641    0.5267


vaf =

    0.7448
```

The partition hierarchy identified is similar to that found for the fixed target `numcltarg6x4`, although there is some minor variation in how the digits 0 and 1 are treated:

Partition	Level Formed (L_2)
{{0,1,2,4,8,3,9,6,5,7}}	.8420
{{0},{1,2,4,8,3,9,6,5,7}}	.7010
{{0},{1},{2,4,8,3,9,6,5,7}}	.6641
{{0},{1},{2,4,8},{3,9,6,5,7}}	.5267
{{0},{1},{2,4,8},{3,9,6},{5,7}}	.4000
{{0},{1},{2,4,8},{3,9,6},{5},{7}}	.3670
{{0},{1},{2},{4,8},{3,9,6},{5},{7}}	.3000
{{0},{1},{2},{4,8},{3,9},{6},{5},{7}}	.2630
{{0},{1},{2},{4,8},{3},{9},{6},{5},{7}}	.2460
{{0},{1},{2},{4},{8},{3},{9},{6},{5},{7}}	—

8.2 Finding Two-Mode Additive Trees

As noted in the introductory material to the current Chapter 8, the identification of a best-fitting two-mode additive tree will be done somewhat differently (because of storage considerations) than for a two-mode ultrametric representation. Specifically, a (two-mode) centroid metric and a (two-mode) ultrametric matrix will be identified so that their sum is a good-fitting two-mode additive tree. Because a centroid metric can be obtained in closed-form, we first illustrate the fitting of just a centroid metric to a two-mode proximity matrix with the m-file, `centfittm.m`. Its usage is of the form

```
[fit,vaf,lengths] = centfittm(proxtm)
```

which gives the least-squares fitted two-mode centroid metric (`FIT`) to `PROXTM`, the two-mode rectangular input proximity matrix (with a dissimilarity interpretation). The n values (where n = number of rows(n_a) + number of columns(n_b)) serve to define the approximating sums, $u_r + v_s$, where the u_r are for the n_a rows and the v_s for the n_b columns; these are given in the vector `LENGTHS` of size $n \times 1$, with row values first followed by the column values. The closed-form formula used for u_r (or v_s) can be given simply as the r^{th} row (or s^{th} column) mean of `PROXTM` minus one-half the grand mean (see Carroll & Pruzansky, 1980, and De Soete et al., 1984, for a further discussion). In the example given below using the two-mode matrix, `number6x4`, a two-mode centroid metric by itself has a vaf of .4737.

```
load number6x4.dat
[fit,vaf,lengths] = centfittm(number6x4)

fit =

    0.7405    0.9101    0.8486    0.8688
    0.5995    0.7691    0.7076    0.7278
    0.4965    0.6661    0.6046    0.6248
    0.3882    0.5579    0.4964    0.5165
    0.4132    0.5829    0.5214    0.5415
    0.4132    0.5829    0.5214    0.5415


vaf =

    0.4737


lengths =

    0.5370
    0.3960
    0.2930
    0.1847
    0.2097
    0.2097
    0.2035
    0.3731
    0.3116
    0.3318
```

The finding of a two-mode additive tree with the m-file, `atreefndtm.m`, proceeds iteratively. A two-mode centroid metric is first found and the original two-mode proximity matrix residualized; a two-mode ultrametric is then identified for the residual matrix. The process repeats with the centroid and ultrametric components alternatingly being refit until a small change in the overall vaf occurs (a value less than 1.0e-006 is used). The m-file has the explicit usage

```
[find,vaf,ultrafit,lengths] = atreefndtm(proxtm,inpermrow,inpermcol)
```

and as noted above, relies on iterative projection heuristically to find a two-mode ultrametric component that is added to a two-mode centroid metric to produce a two-mode additive tree. Here, `PROXTM` is the rectangular input proximity matrix (with a dissimilarity interpretation); `INPERMROW` and `INPERMCOL` are permutations for the row and column objects that determine the order in which the inequality constraints are considered; `FIND` is the found least-squares matrix (with variance-accounted-for of `VAF`) to `PROXTM` satisfying the two-mode additive tree constraints. The vector `LENGTHS` contains the row followed by column values for the two-mode centroid metric component; `ULTRA` is the ultrametric component. In the example given below, the identified two-mode additive-tree for `number6x4` has a vaf of .9053, with a nice structural interpretation of the digits along with some indication now of odd and even digit groupings. The partition hierarchy is reported below the MATLAB output along with an indication of when the various partitions are formed.

```
[find,vaf,ultra,lengths] = atreefndtm(number6x4,randperm(6),randperm(4))

find =

    0.6992    0.9029    0.9104    0.8561
    0.6298    0.6300    0.8411    0.7029
    0.4398    0.8160    0.3670    0.7692
    0.4549    0.5748    0.6661    0.2630
    0.3692    0.7453    0.2460    0.6985
    0.4582    0.4000    0.6694    0.5313


vaf =

    0.9053
```

```
ultra =

    0.1083    0.0520    0.1083    0.0520
    0.1083   -0.1516    0.1083   -0.0318
   -0.0078    0.1083   -0.2919    0.1083
    0.1083   -0.0318    0.1083   -0.2968
   -0.0078    0.1083   -0.3422    0.1083
    0.1083   -0.2099    0.1083   -0.0318


lengths =

    0.4570
    0.3876
    0.3138
    0.2127
    0.2431
    0.2160
    0.1339
    0.3939
    0.3451
    0.3471
```

Partition	Level Formed
{{6,4,8,2,9,3,5,7,1,0}}	.1083
{{6,4,8,2},{9,3,5,7,1,0}}	.0520
{{6,4,8,2},{9,3,5,7,1},{0}}	-.0078
{{6},{4,8,2},{9,3,5,7,1},{0}}	-.0318
{{6},{4,8,2},{9,3},{5,7,1},{0}}	-.1516
{{6},{4,8,2},{9,3},{5,7},{1},{0}}	-.2099
{{6},{4,8,2},{9,3},{5},{7},{1},{0}}	-.2919
{{6},{4,8},{2},{9,3},{5},{7},{1},{0}}	-.2968
{{6},{4,8},{2},{9},{3},{5},{7},{1},{0}}	-.3422
{{6},{4},{8},{2},{9},{3},{5},{7},{1},{0}}	—

8.3 Completing a Two-Mode Ultrametric to one Defined on $S_A \cup S_B$

Instead of relying only on our general intuition (and problem-solving skills) to transform a fitted two-mode ultrametric to one we could interpret directly as a sequence of partitions for the joint set $S_A \cup S_B$, the m-file, `ultracomptm.m`, provides the explicit completion of a given two-mode ultrametric matrix to a symmetric proximity matrix (defined on $S_A \cup S_B$) satisfying the usual ultrametric constraints. The general syntax has the form

```
[ultracomp] = ultracomptm(ultraproxtm)
```

where `ULTRAPROXTM` is the $n_a \times n_b$ fitted two-mode ultrametric matrix, and `ULTRACOMPTM` is the completed $n \times n$ proximity matrix having the usual ultrametric pattern for the complete object set of size $n = n_a + n_b$. As seen in the examples below, the use of `ultrafndtm.m` plus `ultracomptm.m` on the `number6x4` data, and the subsequent application of the `ultraorder.m` routine leads directly to the partition hierarchy we identified earlier:

```
>> load number6x4.dat
>> [find,vaf] = ultrafndtm(number6x4,randperm(6),randperm(4));
>> vaf

vaf =

    0.7448

>> [ultracomp] = ultracomptm(find)

ultracomp =

  Columns 1 through 7

         0    0.8420    0.8420    0.8420    0.8420    0.8420    0.8420
    0.8420         0    0.7010    0.7010    0.7010    0.7010    0.7010
    0.8420    0.7010         0    0.6641    0.3670    0.6641    0.6641
    0.8420    0.7010    0.6641         0    0.6641    0.5267    0.3000
    0.8420    0.7010    0.3670    0.6641         0    0.6641    0.6641
    0.8420    0.7010    0.6641    0.5267    0.6641         0    0.5267
    0.8420    0.7010    0.6641    0.3000    0.6641    0.5267         0
    0.8420    0.7010    0.6641    0.5267    0.6641    0.4000    0.5267
    0.8420    0.7010    0.3670    0.6641    0.2460    0.6641    0.6641
    0.8420    0.7010    0.6641    0.2630    0.6641    0.5267    0.3000

  Columns 8 through 10

    0.8420    0.8420    0.8420
    0.7010    0.7010    0.7010
    0.6641    0.3670    0.6641
    0.5267    0.6641    0.2630
    0.6641    0.2460    0.6641
    0.4000    0.6641    0.5267
    0.5267    0.6641    0.3000
         0    0.6641    0.5267
    0.6641         0    0.6641
    0.5267    0.6641         0

>> [orderprox,orderperm] = ultraorder(ultracomp)

orderprox =

  Columns 1 through 7

         0    0.8420    0.8420    0.8420    0.8420    0.8420    0.8420
    0.8420         0    0.2460    0.3670    0.6641    0.6641    0.6641
    0.8420    0.2460         0    0.3670    0.6641    0.6641    0.6641
    0.8420    0.3670    0.3670         0    0.6641    0.6641    0.6641
    0.8420    0.6641    0.6641    0.6641         0    0.3000    0.3000
    0.8420    0.6641    0.6641    0.6641    0.3000         0    0.2630
    0.8420    0.6641    0.6641    0.6641    0.3000    0.2630         0
    0.8420    0.6641    0.6641    0.6641    0.5267    0.5267    0.5267
    0.8420    0.6641    0.6641    0.6641    0.5267    0.5267    0.5267
    0.8420    0.7010    0.7010    0.7010    0.7010    0.7010    0.7010

  Columns 8 through 10

    0.8420    0.8420    0.8420
    0.6641    0.6641    0.7010
    0.6641    0.6641    0.7010
    0.6641    0.6641    0.7010
    0.5267    0.5267    0.7010
    0.5267    0.5267    0.7010
    0.5267    0.5267    0.7010
         0    0.4000    0.7010
    0.4000         0    0.7010
    0.7010    0.7010         0


orderperm =

     1     9     5     3     7    10     4     8     6     2
```

Similarly, for the two-mode additive tree example, we have the partition hierarchy we gave initially, and what was retrieved immediately from the use of `ultracomptm.m` and `ultraorder.m` on the output ultrametric matrix, `ultra`:

```
>> [find,vaf,ultra,lengths] = atreefndtm(number6x4,randperm(6),randperm(4));
>> vaf

vaf =

    0.9053

>> [ultracomp] = ultracomptm(ultra)

ultracomp =

  Columns 1 through 7

         0    0.0520    0.1083    0.0520    0.1083    0.0520    0.1083
    0.0520         0    0.1083   -0.0318    0.1083   -0.1516    0.1083
    0.1083    0.1083         0    0.1083   -0.2919    0.1083   -0.0078
    0.0520   -0.0318    0.1083         0    0.1083   -0.0318    0.1083
    0.1083    0.1083   -0.2919    0.1083         0    0.1083   -0.0078
    0.0520   -0.1516    0.1083   -0.0318    0.1083         0    0.1083
    0.1083    0.1083   -0.0078    0.1083   -0.0078    0.1083         0
    0.0520   -0.1516    0.1083   -0.0318    0.1083   -0.2099    0.1083
    0.1083    0.1083   -0.2919    0.1083   -0.3422    0.1083   -0.0078
    0.0520   -0.0318    0.1083   -0.2968    0.1083   -0.0318    0.1083

  Columns 8 through 10

    0.0520    0.1083    0.0520
   -0.1516    0.1083   -0.0318
    0.1083   -0.2919    0.1083
   -0.0318    0.1083   -0.2968
    0.1083   -0.3422    0.1083
   -0.2099    0.1083   -0.0318
    0.1083   -0.0078    0.1083
         0    0.1083   -0.0318
    0.1083         0    0.1083
   -0.0318    0.1083         0

>> [orderprox,orderperm] = ultraorder(ultracomp)
```

```
orderprox =

  Columns 1 through 7

         0   -0.0078   -0.0078   -0.0078    0.1083    0.1083    0.1083
   -0.0078         0   -0.3422   -0.2919    0.1083    0.1083    0.1083
   -0.0078   -0.3422         0   -0.2919    0.1083    0.1083    0.1083
   -0.0078   -0.2919   -0.2919         0    0.1083    0.1083    0.1083
    0.1083    0.1083    0.1083    0.1083         0   -0.2968   -0.0318
    0.1083    0.1083    0.1083    0.1083   -0.2968         0   -0.0318
    0.1083    0.1083    0.1083    0.1083   -0.0318   -0.0318         0
    0.1083    0.1083    0.1083    0.1083   -0.0318   -0.0318   -0.1516
    0.1083    0.1083    0.1083    0.1083   -0.0318   -0.0318   -0.1516
    0.1083    0.1083    0.1083    0.1083    0.0520    0.0520    0.0520

  Columns 8 through 10

    0.1083    0.1083    0.1083
    0.1083    0.1083    0.1083
    0.1083    0.1083    0.1083
    0.1083    0.1083    0.1083
   -0.0318   -0.0318    0.0520
   -0.0318   -0.0318    0.0520
   -0.1516   -0.1516    0.0520
         0   -0.2099    0.0520
   -0.2099         0    0.0520
    0.0520    0.0520         0


orderperm =

     7     9     5     3    10     4     2     6     8     1
```

8.3.1 The goldfish_receptor data

To illustrate the results of using our various m-files on the two-mode `goldfish_receptor` data, we give the resulting output below. As to be expected, the various colors are associated with the appropriate cones.

```
>> load goldfish_receptor.dat
>> [find,vaf] = ultrafndtm(goldfish_receptor,randperm(11),randperm(9))

find =
  Columns 1 through 7

   50.0000   50.0000  158.8649  158.8649  158.8649  158.8649  158.8649
   51.5000   51.5000  158.8649  158.8649  158.8649  158.8649  158.8649
   46.0000   47.0000  158.8649  158.8649  158.8649  158.8649  158.8649
  158.8649  158.8649   94.2222   74.6667   46.0000   94.2222  137.8276
  158.8649  158.8649   74.6667   94.2222   94.2222   46.0000  137.8276
  158.8649  158.8649   94.2222   74.6667   48.0000   94.2222  137.8276
  158.8649  158.8649  137.8276  137.8276  137.8276  137.8276   94.2222
  158.8649  158.8649  137.8276  137.8276  137.8276  137.8276   55.0000
  158.8649  158.8649  137.8276  137.8276  137.8276  137.8276   55.0000
  158.8649  158.8649  137.8276  137.8276  137.8276  137.8276   60.0000
  158.8649  158.8649  137.8276  137.8276  137.8276  137.8276   74.6667

  Columns 8 through 9

  158.8649  158.8649
  158.8649  158.8649
  158.8649  158.8649
  137.8276  137.8276
  137.8276  137.8276
  137.8276  137.8276
   94.2222   94.2222
   46.0000   74.6667
   47.0000   74.6667
   60.0000   74.6667
   74.6667   74.6667


vaf =

    0.6209

>> [ultracomp] = ultracomptm(find);
>> [orderprox,orderperm] = ultraorder(ultracomp);

orderprox =

  Columns 1 through 7

         0   47.0000   47.0000   50.0000   51.5000  158.8649  158.8649
   47.0000         0   46.0000   50.0000   51.5000  158.8649  158.8649
   47.0000   46.0000         0   50.0000   51.5000  158.8649  158.8649
   50.0000   50.0000   50.0000         0   51.5000  158.8649  158.8649
   51.5000   51.5000   51.5000   51.5000         0  158.8649  158.8649
  158.8649  158.8649  158.8649  158.8649  158.8649         0   94.2222
  158.8649  158.8649  158.8649  158.8649  158.8649   94.2222         0
  158.8649  158.8649  158.8649  158.8649  158.8649   94.2222   74.6667
  158.8649  158.8649  158.8649  158.8649  158.8649   94.2222   74.6667
  158.8649  158.8649  158.8649  158.8649  158.8649   94.2222   74.6667
  158.8649  158.8649  158.8649  158.8649  158.8649   94.2222   74.6667
  158.8649  158.8649  158.8649  158.8649  158.8649   94.2222   74.6667
  158.8649  158.8649  158.8649  158.8649  158.8649   94.2222   74.6667
  158.8649  158.8649  158.8649  158.8649  158.8649  137.8276  137.8276
  158.8649  158.8649  158.8649  158.8649  158.8649  137.8276  137.8276
  158.8649  158.8649  158.8649  158.8649  158.8649  137.8276  137.8276
  158.8649  158.8649  158.8649  158.8649  158.8649  137.8276  137.8276
  158.8649  158.8649  158.8649  158.8649  158.8649  137.8276  137.8276
  158.8649  158.8649  158.8649  158.8649  158.8649  137.8276  137.8276
  158.8649  158.8649  158.8649  158.8649  158.8649  137.8276  137.8276

  Columns 8 through 14

  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649
  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649
  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649
  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649
  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649
   94.2222   94.2222   94.2222   94.2222   94.2222   94.2222  137.8276
   74.6667   74.6667   74.6667   74.6667   74.6667   74.6667  137.8276
         0   74.6667   74.6667   74.6667   74.6667   74.6667  137.8276
   74.6667         0   46.0000   47.0000   55.0000   60.0000  137.8276
   74.6667   46.0000         0   47.0000   55.0000   60.0000  137.8276
   74.6667   47.0000   47.0000         0   55.0000   60.0000  137.8276
   74.6667   55.0000   55.0000   55.0000         0   60.0000  137.8276
   74.6667   60.0000   60.0000   60.0000   60.0000         0  137.8276
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276         0
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276   46.0000
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276   48.0000
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276   74.6667
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276   94.2222
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276   94.2222
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276   94.2222
```

```
  Columns 15 through 20

  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649
  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649
  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649
  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649
  158.8649  158.8649  158.8649  158.8649  158.8649  158.8649
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276
  137.8276  137.8276  137.8276  137.8276  137.8276  137.8276
   46.0000   48.0000   74.6667   94.2222   94.2222   94.2222
         0   48.0000   74.6667   94.2222   94.2222   94.2222
   48.0000         0   74.6667   94.2222   94.2222   94.2222
   74.6667   74.6667         0   94.2222   94.2222   94.2222
   94.2222   94.2222   94.2222         0   74.6667   74.6667
   94.2222   94.2222   94.2222   74.6667         0   46.0000
   94.2222   94.2222   94.2222   74.6667   46.0000         0


orderperm =

  Columns 1 through 13

    13    12     3     1     2     7    11    20    19     8     9    18    10

  Columns 14 through 20

    16     4     6    15    14     5    17

>> [find,vaf,ultra,lengths] = atreefndtm(goldfish_receptor,randperm(11),randperm(9))

find =

  Columns 1 through 7

   47.0000   53.0000  101.3333  132.0000  171.3608  182.5608  188.2927
   51.4000   51.6000   90.3333  121.0000  160.3608  171.5608  177.2927
   46.4000   46.6000   84.3333  115.0000  154.3608  165.5608  171.2927
  116.3133  116.5133   99.6633   90.4133   50.9000   62.1000   97.4991
  127.1705  127.3705  110.5205  101.2705   49.0000   46.0000  108.3563
  123.6070  123.8070  106.9570   97.7070   87.8609   99.0609   99.1713
  164.2734  164.4734  147.6234  138.3734  128.5273  139.7273   80.0952
  143.5833  143.7833  126.9333  117.6833  107.8372  119.0372   45.1429
  148.7262  148.9262  132.0762  122.8262  112.9801  124.1801   50.2857
  171.8690  172.0690  155.2190  145.9690  136.1229  147.3229   73.4286
  183.5833  183.7833  166.9333  157.6833  147.8372  159.0372   85.1429

  Columns 8 through 9

  216.7498  245.5498
  205.7498  234.5498
  199.7498  228.5498
  125.9563  154.7563
  136.8134  165.6134
  127.6284  156.4284
  108.5524  137.3524
   48.6000   77.4000
   36.1000   64.9000
   58.1000   86.9000
   53.0000   68.0000


vaf =

    0.8663


ultra =

  Columns 1 through 7

 -137.3475 -131.5475  -66.3642  -26.4475   22.7594   22.7594   31.5693
 -121.9475 -121.9475  -66.3642  -26.4475   22.7594   22.7594   31.5693
 -120.9475 -120.9475  -66.3642  -26.4475   22.7594   22.7594   31.5693
   22.7594   22.7594   22.7594   22.7594   -6.9078   -6.9078   31.5693
   22.7594   22.7594   22.7594   22.7594  -19.6650  -33.8650   31.5693
   28.3810   28.3810   28.3810   28.3810   28.3810   28.3810   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693  -24.9848
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693  -39.2471
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693  -39.2471
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693  -39.2471
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693  -39.2471

  Columns 8 through 9

   31.5693   31.5693
   31.5693   31.5693
   31.5693   31.5693
   31.5693   31.5693
   31.5693   31.5693
   31.5693   31.5693
  -24.9848  -24.9848
  -64.2471  -64.2471
  -81.8899  -81.8899
  -83.0328  -83.0328
  -99.8471 -113.6471


lengths =

  111.8748
  100.8748
   94.8748
   21.0812
   31.9383
   22.7533
   60.2313
   39.5413
   44.6841
   67.8270
   79.5413
   72.4727
   72.6727
   55.8227
   46.5727
   36.7267
   47.9267
   44.8487
   73.3058
  102.1058
```

```
>> [ultracomp] = ultracomptm(ultra);

orderprox =

  Columns 1 through 7

         0  -83.0328  -83.0328  -83.0328  -81.8899  -64.2471  -39.2471
  -83.0328         0  -99.8471  -99.8471  -81.8899  -64.2471  -39.2471
  -83.0328  -99.8471         0 -113.6471  -81.8899  -64.2471  -39.2471
  -83.0328  -99.8471 -113.6471         0  -81.8899  -64.2471  -39.2471
  -81.8899  -81.8899  -81.8899  -81.8899         0  -64.2471  -39.2471
  -64.2471  -64.2471  -64.2471  -64.2471  -64.2471         0  -39.2471
  -39.2471  -39.2471  -39.2471  -39.2471  -39.2471  -39.2471         0
  -24.9848  -24.9848  -24.9848  -24.9848  -24.9848  -24.9848  -24.9848
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693

  Columns 8 through 14

  -24.9848   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
  -24.9848   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
  -24.9848   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
  -24.9848   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
  -24.9848   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
  -24.9848   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
  -24.9848   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
         0   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693         0  -26.4475  -26.4475  -26.4475  -26.4475  -26.4475
   31.5693  -26.4475         0  -66.3642  -66.3642  -66.3642  -66.3642
   31.5693  -26.4475  -66.3642         0 -131.5475 -131.5475 -121.9475
   31.5693  -26.4475  -66.3642 -131.5475         0 -137.3475 -121.9475
   31.5693  -26.4475  -66.3642 -131.5475 -137.3475         0 -121.9475
   31.5693  -26.4475  -66.3642 -121.9475 -121.9475 -121.9475         0
   31.5693  -26.4475  -66.3642 -120.9475 -120.9475 -120.9475 -120.9475
   31.5693   22.7594   22.7594   22.7594   22.7594   22.7594   22.7594
   31.5693   22.7594   22.7594   22.7594   22.7594   22.7594   22.7594
   31.5693   22.7594   22.7594   22.7594   22.7594   22.7594   22.7594
   31.5693   22.7594   22.7594   22.7594   22.7594   22.7594   22.7594
   31.5693   28.3810   28.3810   28.3810   28.3810   28.3810   28.3810

  Columns 15 through 20

   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
   31.5693   31.5693   31.5693   31.5693   31.5693   31.5693
  -26.4475   22.7594   22.7594   22.7594   22.7594   28.3810
  -66.3642   22.7594   22.7594   22.7594   22.7594   28.3810
 -120.9475   22.7594   22.7594   22.7594   22.7594   28.3810
 -120.9475   22.7594   22.7594   22.7594   22.7594   28.3810
 -120.9475   22.7594   22.7594   22.7594   22.7594   28.3810
 -120.9475   22.7594   22.7594   22.7594   22.7594   28.3810
         0   22.7594   22.7594   22.7594   22.7594   28.3810
   22.7594         0   -6.9078   -6.9078   -6.9078   28.3810
   22.7594   -6.9078         0  -33.8650  -19.6650   28.3810
   22.7594   -6.9078  -33.8650         0  -19.6650   28.3810
   22.7594   -6.9078  -19.6650  -19.6650         0   28.3810
   28.3810   28.3810   28.3810   28.3810   28.3810         0


orderperm =

  Columns 1 through 13

    10    19    20    11     9     8    18     7    15    14    13    12     1

  Columns 14 through 20

     2     3     4    17     5    16     6
```

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Part III

The Representation of Proximity Matrices by Structures Dependent on Order (Only)

An Introduction to Order-Theoretic Representational Structures

Nonmetric multidimensional scaling (NMDS) as developed by Shepard (1962a,b) and Kruskal (1964a,b), has become a very familiar method in the psychological research literature for representing structure that may be inherent among a set of objects. Judging by the number of published substantive applications, whenever data are given in the form of a symmetric proximity matrix containing numerical relationship information between distinct object pairs, NMDS may have now become the default method of analysis. This routine use of NMDS, however, when faced with elucidating whatever pattern of relationships may underly a given set of proximities, does have interpretive implications and consequences. For one, there is an implicit choice made that whatever major generality will be allowed should reside primarily in the particular proximities being fitted by the explicitly parameterized (Euclidean) spatial structure. Thus, an optimal (usually monotonic) transformation of the proximities is sought in conjunction with the construction of a spatial representation. Second, the parameterized spatial structure implicitly involves fitting the (transformed) proximities by some function of the differences in object placement along a set of coordinate axes that may be best suited for representing object variation that could, at least in theory, be allowed to vary continuously. For instance, in the common Euclidean model we use the square root of the sum of squared coordinate differences along a set of axes (although the particular axis system selected is open to some arbitrariness). The tacit implication is that if the structure underlying the proximities is more classificatory (and discrete) in nature, we may not do well in representing it by a spatial model that should do much better in the presence of more continuous variation (cf. Pruzansky, Tversky, and Carroll, 1982). In fact, in the limiting case where there exists a partition of the object set in which all proximities for object pairs within an object class are smaller than for object pairs between classes (and where proximities are keyed as dissimilarities so that larger values represent more dissimilar objects), NMDS will typically give a degenerate representation in which all objects within each class are located at the same spatial location and the optimally transformed proximities consist of just two values, one for the within-class proximities and one for the between-class proximities (cf. Shepard, 1974).

This part of the book concentrates on an alternative approach to understanding what a given proximity matrix may be depicting about the objects on which it was constructed, and one that does not require a prior commitment to the sole use of either some form of dimensional model (as in NMDS), or one that is strictly classificatory (as in the use of a partition hierarchy and the implicit fitting of an ultrametric that serves as the representational mechanism for the hierarchical clustering). The method of analysis is based on approximating a given proximity matrix additively by a sum of matrices, where each component in the sum is subject to specific patterning restrictions on its entries. The restrictions imposed on each component of the decomposition (to be referred to as matrices with anti-Robinson forms) are very general and encompass interpretations that might be dimensional, or classificatory, or some combination of both (e.g., through object classes that are themselves placed dimensionally in some space). Thus, as one special case — and particularly when an (optimal) transformation of the proximities is also permitted (as we will generally allow), proximity matrices that are well interpretable through NMDS should also be interpretable through an additive decomposition of the (transformed) proximity matrix. Alternatively, when classificatory structures of various kinds might underlie a set of proximities (and the direct use of NMDS could possibly lead to a degeneracy), additive decompositions may still provide an analysis strategy for elucidating the structure.

The algorithmic details of fitting to a given proximity matrix a sum of matrices each having the desired general patterning to its entries (or even more explicitly parameterized forms that may be of help in providing a detailed interpretation, such as those given by partition hierarchies or unidimensional scales), are available in a series of papers that have appeared in the literature (i.e., Hubert and Arabie, 1994, 1995; Hubert, Arabie, and Meulman, 1997, 1998). Thus, in this sequel we can merely refer to these sources for the actual mechanics of carrying out the various decompositions. More unique aspects that will be incorporated in the documentation to follow are (a) the possible integration of (optimal) transformations for use with the originally given proximities to be fit by an additive matrix decomposition, and (b) the fitting of more restrictive parameterized forms to the various components of a decomposition in attempting to give a detailed substantive interpretation of what each separate matrix in the decomposition may be depicting. In this latter instance, one of our concerns might be directed toward the issue of whether a particular matrix as part of a decomposition is indicating primarily dimensional or classificatory aspects of the original proximities (or possibly and what may be more typical, some combination of the two). In these latter cases, the m-files discussed as part of the documentation given in the earlier parts of this book for Linear Unidimensional Scaling and for the fitting of Tree Structures are particularly relevant.

Chapter 9

Anti-Robinson (AR) Matrices for Symmetric Proximity Data

Denoting an arbitrary symmetric $n \times n$ matrix by $\mathbf{A} = \{a_{ij}\}$, where the main diagonal entries are considered irrelevant and assumed to be zero (i.e., $a_{ii} = 0$ for $1 \leq i \leq n$), $\mathbf{A}$ is said to have an anti-Robinson (AR) form if after some reordering of the rows and columns of $\mathbf{A}$, the entries within each row and column have a distinctive pattern: moving away from the zero main diagonal entry within any row or any column, the entries never decrease. Generally, matrices having AR forms can appear both in spatial representations for a set of proximities as functions of the absolute differences in coordinate values along some axis, or for classificatory structures that are characterized through an ultrametric.

To illustrate, we first let $\mathbf{P} = \{p_{ij}\}$ be a given $n \times n$ proximity (dissimilarity) matrix among the n objects in a set $S = \{O_1, O_2, \ldots, O_n\}$ (where $p_{ii} = 0$ for $1 \leq i \leq n$). Then, suppose, for example, a two-dimensional Euclidean representation is possible for $\mathbf{P}$ and its entries are very well representable by the distances in this space, so

$$p_{ij} \approx \sqrt{(x_{1i} - x_{1j})^2 + (x_{2i} - x_{2j})^2} \ ,$$

where x_{ki} and x_{kj} are the coordinates on the k^{th} axis (for $k = 1$ and 2) for objects O_i and O_j (and the symbol $\approx$ is used to indicate approximation). Here, a simple monotonic transformation (squaring) of the proximities should then be fit well by the sum of two matrices both having AR forms, i.e.,

$$\{p_{ij}^2\} \approx \{(x_{1i} - x_{1j})^2\} + \{(x_{2i} - x_{2j})^2\}.$$

In a classificatory framework, if $\{p_{ij}\}$ were well representable, say, as a sum of two matrices, $\mathbf{A}_1 = \{a_{ij}^{(1)}\}$ and $\mathbf{A}_2 = \{a_{ij}^{(2)}\}$, each satisfying the ultrametric inequality, i.e., $a_{ij}^{(k)} \leq \max\{a_{ih}^{(k)}, a_{hj}^{(k)}\}$ for $k = 1$ and 2, then

$$\{p_{ij}\} \approx \{a_{ij}^{(1)}\} + \{a_{ij}^{(2)}\},$$

and each of the constituent matrices can be reordered to display an AR form. As can be seen in Part II of this manual, any matrix whose entries satisfy the ultrametric inequality can be represented by a sequence of partitions that are hierarchically related.

Given some proximity matrix $\mathbf{P}$, the task of approximating it as a sum of matrices each having an AR form is implemented through an iterative optimization strategy based on a least-squares loss criterion that is discussed in detail by Hubert and Arabie (1994). Given the manner in which the optimization process is carried out sequentially, each successive AR matrix in any decomposition generally accounts for less and less of the patterning of the original proximity information (and very analogous to what is typically observed in a principal component decomposition of a covariance matrix). In fact, it has been found empirically that for the many data sets we have analyzed, only a very small number of such AR matrices are ever necessary to represent almost all of the patterning in the given proximities. As a succinct summary that we could give to this empirical experience: no more than three AR matrices are ever necessary; the data analyst can usually get by with two; and sometimes one will suffice.

The substantive challenge that remains, once a well-fitting decomposition is found for a given proximity matrix, is to interpret substantively what each term in the decomposition might be depicting. The strategy that could be followed would approximate each separate AR matrix by ones having a more restrictive form, and usually those representing some type of unidimensional scale (from Part I) or partition hierarchy (from Part II). As one aspect of this interpretive process, an evaluation could be made of the degree to which classificatory or dimensional interpretations may best represent each AR matrix in the given decomposition.

9.0.2 Incorporating Transformations

One generalization that we will now allow to what has already been discussed in the literature for fitting sums of AR matrices to a proximity matrix $\mathbf{P}$, is the possible inclusion of an (optimal) transformation of the proximities. Thus, instead of just representing $\mathbf{P}$ as a sum of K matrices (and generally, for K very small) that we might denote as $\mathbf{A}_1 + \cdots + \mathbf{A}_K$, where each $\mathbf{A}_k$, $1 \le k \le K$, has an AR form, an (optimally) transformed matrix $\tilde{\mathbf{P}} = \{\tilde{p}_{ij}\}$ will be fitted by such a sum, say, $\tilde{\mathbf{A}}_1 + \cdots + \tilde{\mathbf{A}}_K$, where the entries in $\tilde{\mathbf{P}}$ are monotonic with respect to those in $\mathbf{P}$, i.e., for all $O_i, O_j, O_k, O_l \in S$, $p_{ij} < p_{kl} \Rightarrow \tilde{p}_{ij} \le \tilde{p}_{kl}$. In the sequel we will rely on the m-file, `proxmon.m`, documented in Part I, which constructs optimal monotonic transformations by the same method of isotonic regression commonly used in NMDS (i.e., Kruskal's [1964a,b] primary approach to tied proximities in $\mathbf{P}$ that are allowed to be untied after transformation). Such transformations, for example, form the default option in the implementation of NMDS in the program KYST-2A (Kruskal, Young, and Seery, 1977) and in SYSTAT (Wilkinson, 1988).

The process of finding $\tilde{\mathbf{P}}$ and $\tilde{\mathbf{A}}_1 + \cdots + \tilde{\mathbf{A}}_K$ proceeds iteratively, with the original proximity matrix $\mathbf{P}$ first fit by $\mathbf{A}_1 + \cdots + \mathbf{A}_K$; a subsequent optimal (monotonic) transformation of $\mathbf{P}$ (through a least-squares approximation to $\mathbf{A}_1 + \cdots + \mathbf{A}_K$) is identified, which is then refitted by the matrix sum. In many cases, this whole process can now be cycled through iteratively until convergence, i.e., through a sequential fitting and refitting of the optimally transformed proximities and its representation as a sum of matrices each having an AR form. In some contexts, however (particularly when fitting a single AR matrix [i.e., when $K = 1$]), it is probably best not to proceed to a complete convergence but instead to terminate the process after only a single optimal monotonic transformation of $\mathbf{P}$ is identified and then to refit by a matrix sum. This usage will be referred to as a single iteration optimal transformation (SIOT). If carried through to convergence, a perfect representation may be obtained but only at the expense of losing almost all the patterning contained within the original proximity matrix. For example, in fitting a single AR matrix, the optimal transformation identified after convergence might consist of just two values, with one corresponding to the smallest proximity in the original matrix and all others equal. Although technically permissible since this situation does reflect a perfect AR form, most of the detail present in the original proximity matrix is also lost. Difficulties with such so-called degeneracies have been pointed out by Carroll (1992), particularly when faced with fitting classificatory structures to a given proximity matrix.

9.0.3 Interpreting the Structure of an AR matrix

In representing a proximity matrix $\mathbf{P}$ as a sum, $\mathbf{A}_1 + \cdots + \mathbf{A}_K$ (or an optimal transformation $\tilde{\mathbf{P}}$ as $\tilde{\mathbf{A}}_1 + \cdots + \tilde{\mathbf{A}}_K$), the interpretive task remains to explain substantively what each term of the decomposition might be depicting. We suggest four possible strategies below, with the first two attempting to understand the structure of an AR matrix directly and without much loss of detail; the last two require the imposition of strictly parameterized approximations in the form of either an ultrametric or a unidimensional scale. In the discussion below, $\mathbf{A} = \{a_{ij}\}$ will be assumed to have an AR form that is displayed by the given row and column order.

(A) Complete representation and reconstruction through a collection of subsets and associated subset diameters:

The entries in any AR matrix $\mathbf{A}$ can be reconstructed exactly through a collection of M subsets of the original object set $S = \{O_1, \ldots, O_n\}$, denoted by $S_1, \ldots, S_M$, and where M is determined by the particular pattern of tied entries, if any, in $\mathbf{A}$. These M subsets have the following characteristics:

(i) each S_m, $1 \leq m \leq M$, consists of a sequence of (two or more) consecutive integers so that $M \leq n(n-1)/2$. (This bound holds because the number of different subsets having consecutive integers for any given fixed ordering is $n(n-1)/2$, and will be achieved if all the entries in the AR matrix $\mathbf{A}$ are distinct).

(ii) each S_m, $1 \leq m \leq M$, has a diameter, denoted by $d(S_m)$, so that for all object pairs within S_m, the corresponding entries in $\mathbf{A}$ are less than or equal to the diameter. The subsets, $S_1, \ldots, S_M$, can be assumed ordered as $d(S_1) \leq d(S_2) \leq \cdots \leq d(S_M)$, and if $S_m \subseteq S_{m'}$, $d(S_m) \leq d(S_{m'})$.

(iii) each entry in $\mathbf{A}$ can be reconstructed from $d(S_1), \ldots, d(S_M)$, i.e., for $1 \leq i, j \leq n$,

$$a_{ij} = \min_{1 \leq m \leq M} \{d(S_m) \mid O_i, O_j \in S_m\},$$

so the minimum diameter for subsets containing an object pair $O_i, O_j \in S$ is equal to a_{ij}. Given $\mathbf{A}$, the collection of subsets $S_1, \ldots, S_M$ and their diameters can be identified by inspection through the use of an increasing threshold that starts from the smallest entry in $\mathbf{A}$, and observing which subsets containing contiguous objects emerge from this process. The substantive interpretation of what $\mathbf{A}$ is depicting reduces to explaining why those subsets with the smallest diameters are so homogenous. For convenience of reference, the subsets $S_1, \ldots, S_M$ will be referred to as the set of AR reconstructive subsets.

(B) Representation by a strongly anti-Robinson matrix:

If the matrix $\mathbf{A}$ has a somewhat more restrictive form than just being AR, and is also *strongly* anti-Robinson, a convenient graphical representation can be given to the collection of AR reconstructive subsets $S_1, \ldots, S_M$ and their diameters, and how they can serve to retrieve $\mathbf{A}$. Specifically, $\mathbf{A}$ is said to be strongly anti-Robinson (SAR) if (considering the above-diagonal entries of $\mathbf{A}$) whenever two entries in adjacent columns are equal ($a_{ij} = a_{i(j+1)}$), those in the same two adjacent columns in the previous row are also equal ($a_{(i-1)j} = a_{(i-1)(j+1)}$ for $1 \leq i-1 < j \leq n-1$); also, whenever two entries in adjacent rows are equal ($a_{ij} = a_{(i+1)j}$), those in the same two adjacent rows in the succeeding column are also equal ($a_{i(j+1)} = a_{(i+1)(j+1)}$ for $2 \leq i+1 < j \leq n-1$).

When $\mathbf{A}$ is SAR, the collection of subsets, $S_1, \ldots, S_M$, and their diameters, and how these serve to reconstruct $\mathbf{A}$ can be modeled graphically as we will see in Section 9.5. The internal nodes (represented by solid circles) in each of these figures are at a height equal to the diameter of the respective subset; the consecutive objects forming that subset are identifiable by downward paths from the internal nodes to the terminal nodes corresponding to the objects in $S = \{O_1, \ldots, O_n\}$ (represented by labeled open circles). An entry a_{ij} in $\mathbf{A}$ can be reconstructed as the minimum node height of a subset for which a path can be constructed from O_i up to that internal node and then back down to O_j. (To prevent undue graphical "clutter", only the most homogenous subsets from $S_1, \ldots, S_M$ having the smallest diameters should actually be included in the graphical representation of an SAR matrix; each figure would explicitly show only how the smallest entries in $\mathbf{A}$ can be reconstructed, although each could be easily extended to include all of $\mathbf{A}$. The calibrated vertical axis in such figures could routinely include the heights at which the additional internal nodes would have to be placed to effect such a complete reconstruction.)

Given an arbitrary AR matrix $\mathbf{A}$, a least-squares SAR approximating matrix to $\mathbf{A}$ can be found using the heuristic optimization search strategy illustrated in Section 9.3 and developed in Hubert, Arabie, and Meulman (1998). This latter source also discusses in detail (through counterexample) why strongly AR conditions need to be imposed to obtain a consistent graphical representation.

(C) Representation by a unidimensional scale:

To obtain greater graphical simplicity for an eventual substantive interpretation than offered by an SAR matrix, one possibility is to use approximating unidimensional scales. To be explicit, one very simple form that an AR matrix $\mathbf{A}$ may assume is interpretable by a single dimension and through a unidimensional scale in which the entries have the parameterized form, $\mathbf{A} = \{a_{ij}\} = \{| x_j - x_i | + c\}$, where the coordinates are ordered as $x_1 \leq x_2 \leq \cdots \leq x_n$ and c is an estimated constant. Given any proximity matrix, a least-squares approximating unidimensional scale can be obtained through the optimization strategies of Part I, and would be one (dimensional) method that could be followed in attempting to interpret what a particular AR component of a decomposition might be revealing.

(D) Representation by an ultrametric:

A second simple form that an AR matrix $\mathbf{A}$ could have is strictly classificatory in which the entries in $\mathbf{A}$ satisfy the ultrametric condition: $a_{ij} \leq \max\{a_{ik}, a_{jk}\}$ for all $O_i, O_j, O_k \in S$. As a threshold is increased from the smallest entry in $\mathbf{A}$, a sequence of partitions of S is identified in which each partition is constructed from the previous one by uniting pairs of subsets from the latter. A partition identified at a given threshold level has equal values in $\mathbf{A}$ between each given pair of subsets, and all the within subset values are not greater than the between subset values. The reconstructive subsets $S_1, \ldots, S_M$ that would represent the AR matrix $\mathbf{A}$ are now the new subsets that are formed in the sequence of partitions, and have the property that if $d(S_m) \leq d(S_{m'})$, then $S_m \subseteq S_{m'}$ or $S_m \cap S_{m'} = \oslash$. Given any proximity matrix, a least-squares approximating ultrametric can be constructed by the heuristic optimization routines developed in Part II, and would be another (classificatory) strategy for interpreting what a particular AR component of a decomposition might be depicting. As might be noted, there are generally $n - 1$ subsets (each of size greater than one) in the collection of reconstructive subsets for any ultrametric, and thus $n - 1$ values need to be estimated in finding the least-squares approximation (which is the same number needed for a least-squares approximating unidimensional scale, based on obtaining the $n-1$ nonnegative separation values between x_i and x_{i+1} for $1 \leq i \leq n - 1$).

9.1 Fitting a Given AR Matrix in the L_2-Norm

The MATLAB function m-file, `arobfit.m`, fits an anti-Robinson matrix using iterative projection to a symmetric proximity matrix in the L_2-norm. The usage syntax is of the form

```
[fit,vaf] = arobfit(prox,inperm)
```

where `PROX` is the input proximity matrix ($n \times n$ with a zero main diagonal and a dissimilarity interpretation); `INPERM` is a given permutation of the first n integers; `FIT` is the least-squares optimal matrix (with variance-accounted-for of `VAF`) to `PROX` having an anti-Robinson form for the row and column object ordering given by `INPERM`. A recording of a MATLAB session using the `number.dat` data file and object ordering given by the identity permutation follows:

```
load number.dat
```

```
inperm = 1:10

inperm =

     1     2     3     4     5     6     7     8     9    10

[fit,vaf] = arobfit(number,inperm)

fit =

  Columns 1 through 7

         0    0.4210    0.5840    0.6965    0.6965    0.7960    0.7960
    0.4210         0    0.2840    0.3460    0.6170    0.6170    0.6940
    0.5840    0.2840         0    0.2753    0.2753    0.5460    0.5460
    0.6965    0.3460    0.2753         0    0.2753    0.3844    0.3844
    0.6965    0.6170    0.2753    0.2753         0    0.3844    0.3844
    0.7960    0.6170    0.5460    0.3844    0.3844         0    0.3844
    0.7960    0.6940    0.5460    0.3844    0.3844    0.3844         0
    0.8600    0.6940    0.5853    0.5853    0.5530    0.4000    0.3857
    0.8600    0.7413    0.5853    0.5853    0.5530    0.5530    0.3857
    0.8600    0.7413    0.7413    0.5853    0.5853    0.5853    0.3857

  Columns 8 through 10

    0.8600    0.8600    0.8600
    0.6940    0.7413    0.7413
    0.5853    0.5853    0.7413
    0.5853    0.5853    0.5853
    0.5530    0.5530    0.5853
    0.4000    0.5530    0.5853
    0.3857    0.3857    0.3857
         0    0.3857    0.3857
    0.3857         0    0.3857
    0.3857    0.3857         0


vaf =

    0.6979
```

9.1.1 Fitting the (In)-equality Constraints Implied by a Given Matrix in the L_2 Norm

At times it may be useful to fit through iterative projection a given set of equality and inequality constraints (as represented by the equalities and inequalities present among the entries in a given target matrix) to a symmetric proximity matrix in the L_2-norm. If the target matrix is AR in form already, the resulting fitted matrix would also AR in form, but the m-function, `targfit.m`, could be used more generally with any chosen target matrix. The usage follows the form

```
[fit,vaf] = targfit(prox,targ)
```

where, as usual, `PROX` is the input proximity matrix (with a zero main diagonal and a dissimilarity interpretation); `TARG` is a matrix of the same size as `PROX`; `FIT` is the least-squares optimal matrix (with variance-accounted-for of `VAF`) to `PROX` satisfying the equality and inequality constraints implicit among all the entries in `TARG`. An example follows in which the given target matrix is a distance matrix (having an AR form) between equally-spaced object placements along a line; the resulting fitted matrix obviously has an AR form as well:

```
load number.dat
[prox10 targlin targcir] = ransymat(10);
targlin

targlin =

     0     1     2     3     4     5     6     7     8     9
     1     0     1     2     3     4     5     6     7     8
     2     1     0     1     2     3     4     5     6     7
     3     2     1     0     1     2     3     4     5     6
     4     3     2     1     0     1     2     3     4     5
     5     4     3     2     1     0     1     2     3     4
     6     5     4     3     2     1     0     1     2     3
     7     6     5     4     3     2     1     0     1     2
     8     7     6     5     4     3     2     1     0     1
     9     8     7     6     5     4     3     2     1     0

[fit,vaf] = targfit(number,targlin)

fit =

  Columns 1 through 7

         0    0.3714    0.3714    0.5363    0.5363    0.6548    0.6548
```

```
    0.3714         0    0.3714    0.3714    0.5363    0.5363    0.6548
    0.3714    0.3714         0    0.3714    0.3714    0.5363    0.5363
    0.5363    0.3714    0.3714         0    0.3714    0.3714    0.5363
    0.5363    0.5363    0.3714    0.3714         0    0.3714    0.3714
    0.6548    0.5363    0.5363    0.3714    0.3714         0    0.3714
    0.6548    0.6548    0.5363    0.5363    0.3714    0.3714         0
    0.7908    0.6548    0.6548    0.5363    0.5363    0.3714    0.3714
    0.7908    0.7908    0.6548    0.6548    0.5363    0.5363    0.3714
    0.8500    0.7908    0.7908    0.6548    0.6548    0.5363    0.5363

  Columns 8 through 10

    0.7908    0.7908    0.8500
    0.6548    0.7908    0.7908
    0.6548    0.6548    0.7908
    0.5363    0.6548    0.6548
    0.5363    0.5363    0.6548
    0.3714    0.5363    0.5363
    0.3714    0.3714    0.5363
         0    0.3714    0.3714
    0.3714         0    0.3714
    0.3714    0.3714         0


vaf =

    0.5105
```

9.2 Finding an AR Matrix in the L_2-Norm

The *fitting* of a given AR matrix by the m-function of Section 9.1, `arobfit.m`, requires the presence of a beginning permutation to direct the optimization process. Thus, the *finding* of a best-fitting AR matrix reduces to the identification of an appropriate object permutation to use in the first place. We suggest the adoption of `order.m`, which carries out an iterative Quadratic Assignment maximization task using a given square ($n \times n$) proximity matrix `PROX` (with a zero main diagonal and a dissimilarity interpretation). Three separate local operations are used to permute the rows and columns of the proximity matrix to maximize the cross-product index with respect to a given square target matrix `TARG`: pairwise interchanges of objects in the permutation defining the row and column order of the square proximity matrix; the insertion of from 1 to `KBLOCK` (which is less than or equal to $n-1$) consecutive objects in the permutation defining the row and column order of the data matrix; the rotation of from 2 to `KBLOCK` (which is less than or equal to $n-1$) consecutive objects in the permutation defining the row and column order of the data matrix. The usage syntax has the form

```
[outperm,rawindex,allperms,index] =  order(prox,targ,inperm,kblock)
```

where `INPERM` is the input beginning permutation (a permutation of the first n integers); `OUTPERM` is the final permutation of `PROX` with the cross-product index `RAWINDEX` with respect to `TARG`. The cell array `ALLPERMS` contains `INDEX` entries corresponding to all the permutations identified in the optimization from `ALLPERMS{1}` = `INPERM` to `ALLPERMS{INDEX}` = `OUTPERM`.

A recording of a MATLAB session using `order.m` is listed below with the beginning `INPERM` given as the identity permutation, `TARG` by an equally-spaced object placement along a line, and `KBLOCK` set at 3. Based upon the generated `OUTPERM`, `arobfit.m` is then invoked to fit an AR form having final `VAF` of .7782.

```
load number.dat
[prox10,targlin,targcir] = ransymat(10);
[outperm,rawindex,allperms,index] =  order(number,targlin,1:10,3)

outperm =

     1     2     3     5     4     6     7     9    10     8


rawindex =

  206.4920


allperms =

    [1x10 double]    [1x10 double]    [1x10 double]    [1x10 double]


index =

     4

[fit, vaf] = arobfit(number, outperm)

fit =

  Columns 1 through 7
```

```
         0    0.4210    0.5840    0.6840    0.7090    0.7960    0.7960
    0.4210         0    0.2840    0.4960    0.4960    0.5880    0.7357
    0.5840    0.2840         0    0.0590    0.3835    0.4928    0.4928
    0.6840    0.4960    0.0590         0    0.3835    0.3985    0.3985
    0.7090    0.4960    0.3835    0.3835         0    0.3750    0.3750
    0.7960    0.5880    0.4928    0.3985    0.3750         0    0.3750
    0.7960    0.7357    0.4928    0.3985    0.3750    0.3750         0
    0.8210    0.7357    0.4928    0.4928    0.4928    0.4928    0.3460
    0.8500    0.7357    0.7357    0.6830    0.4928    0.4928    0.3460
    0.9090    0.7357    0.7357    0.7357    0.5920    0.4928    0.4253

  Columns 8 through 10

    0.8210    0.8500    0.9090
    0.7357    0.7357    0.7357
    0.4928    0.7357    0.7357
    0.4928    0.6830    0.7357
    0.4928    0.4928    0.5920
    0.4928    0.4928    0.4928
    0.3460    0.3460    0.4253
         0    0.3460    0.4253
    0.3460         0    0.4253
    0.4253    0.4253         0


vaf =

    0.7782
```

The m-file, `arobfnd.m` is our preferred method for actually identifying a single AR form. It incorporates an initial equally-spaced target and uses the iterative QA routine of `order.m` to generate better permutations; the obtained AR forms then are used as new targets against which possibly even better permutations might be identified, until convergence (i.e., the identified permutations remain the same). The syntax is as follows:

```
[fit, vaf, outperm] = arobfnd(prox, inperm, kblock)
```

where `PROX` is the input proximity matrix ($n \times n$ with a zero main diagonal and a dissimilarity interpretation); `INPERM` is a given starting permutation of the first n integers; `FIT` is the least-squares optimal matrix (with variance-accounted-for of `VAF`) to `PROX` having an anti-Robinson form for the row and column object ordering given by the ending permutation `OUTPERM`; `KBLOCK` defines the block size in the use the iterative quadratic assignment routine.

As seen from the example below, and starting from a random initial permutation, the same AR form is found as with just one application of `order.m` reported above.

```
[fit, vaf, outperm] = arobfnd(number, randperm(10), 1)

fit =

  Columns 1 through 7

         0    0.4253    0.4253    0.4253    0.4928    0.5920    0.7357
    0.4253         0    0.3460    0.3460    0.4928    0.4928    0.6830
    0.4253    0.3460         0    0.3460    0.4928    0.4928    0.4928
    0.4253    0.3460    0.3460         0    0.3750    0.3750    0.3985
    0.4928    0.4928    0.4928    0.3750         0    0.3750    0.3985
    0.5920    0.4928    0.4928    0.3750    0.3750         0    0.3835
    0.7357    0.6830    0.4928    0.3985    0.3985    0.3835         0
    0.7357    0.7357    0.4928    0.4928    0.4928    0.3835    0.0590
    0.7357    0.7357    0.7357    0.7357    0.5880    0.4960    0.4960
    0.9090    0.8500    0.8210    0.7960    0.7960    0.7090    0.6840

  Columns 8 through 10

    0.7357    0.7357    0.9090
    0.7357    0.7357    0.8500
    0.4928    0.7357    0.8210
    0.4928    0.7357    0.7960
    0.4928    0.5880    0.7960
    0.3835    0.4960    0.7090
    0.0590    0.4960    0.6840
         0    0.2840    0.5840
    0.2840         0    0.4210
    0.5840    0.4210         0


vaf =

    0.7782


outperm =

     8    10     9     7     6     4     5     3     2     1
```

9.3 Fitting and Finding a Strongly Anti-Robinson (SAR) Matrix in the L_2-Norm

The two m-functions, (`sarobfit.m`) and (`sarobfnd.m`), are direct analogues of `arobfit.m` and `arobfnd.m`, respectively, but are concerned with fitting and finding *strongly* anti-Robinson forms. The syntax for `sarobfit.m`, which fits a strongly anti-Robinson matrix using iterative projection to a symmetric proximity matrix in the L_2-norm, is

```
[fit, vaf] = sarobfit(prox, inperm)
```

where, again, `PROX` is the input proximity matrix ($n \times n$ with a zero main diagonal and a dissimilarity interpretation); `INPERM` is a given permutation of the first n integers; `FIT` is the least-squares optimal matrix (with variance-accounted-for of `VAF`) to `PROX` having a strongly anti-Robinson form for the row and column object ordering given by `INPERM`.

An example follows using the same identity permutation as was done in fitting an AR form with `arobfit.m`; as might be expected from using the more restrictive strongly anti-Robinson form, the variance-accounted-for drops to .6128 from .6979.

```
load number.dat
[fit,vaf] = sarobfit(number,1:10)

fit =

  Columns 1 through 7

         0    0.4210    0.5840    0.6965    0.6965    0.7960    0.7960
    0.4210         0    0.2840    0.4960    0.4960    0.6730    0.6730
    0.5840    0.2840         0    0.2753    0.2753    0.4553    0.4553
    0.6965    0.4960    0.2753         0    0.2753    0.4553    0.4553
    0.6965    0.4960    0.2753    0.2753         0    0.3977    0.3977
    0.7960    0.6730    0.4553    0.4553    0.3977         0    0.3977
    0.7960    0.6730    0.4553    0.4553    0.3977    0.3977         0
    0.8600    0.6820    0.6050    0.6050    0.5557    0.5557    0.3857
    0.8600    0.6820    0.6050    0.6050    0.5557    0.5557    0.3857
    0.8600    0.6820    0.6050    0.6050    0.5557    0.5557    0.3857

  Columns 8 through 10

    0.8600    0.8600    0.8600
    0.6820    0.6820    0.6820
    0.6050    0.6050    0.6050
    0.6050    0.6050    0.6050
    0.5557    0.5557    0.5557
    0.5557    0.5557    0.5557
    0.3857    0.3857    0.3857
         0    0.3857    0.3857
    0.3857         0    0.3857
    0.3857    0.3857         0


vaf =

    0.6128
```

The m-function `sarobfnd.m`, which fits a strongly anti-Robinson matrix using iterative projection to a symmetric proximity matrix in the L_2-norm based on a permutation identified through the use of iterative quadratic assignment, has the expected syntax

```
[fit, vaf, outperm] = sarobfnd(prox, inperm, kblock)
```

where, again, `PROX` is the input proximity matrix ($n \times n$ with a zero main diagonal and a dissimilarity interpretation); `INPERM` is a given starting permutation of the first n integers; `FIT` is the least-squares optimal matrix (with variance-accounted-for of `VAF`) to `PROX` having a strongly anti-Robinson form for the row and column object ordering given by the ending permutation `OUTPERM`. As usual, `KBLOCK` defines the block size in the use the iterative quadratic assignment routine.

In the MATLAB recording below, and starting from a random permutation, a strongly anti-Robinson form is found with a variance-accounted-for of .7210 (and is an expected drop from the value of .7782 for the anti-Robinson form found using `arobfnd.m`).

```
[fit,vaf,outperm] = sarobfnd(number,randperm(10),1)

fit =

  Columns 1 through 7

         0    0.4210    0.5840    0.6965    0.6965    0.7960    0.7960
    0.4210         0    0.2840    0.4960    0.4960    0.6730    0.6730
    0.5840    0.2840         0    0.0590    0.3835    0.4723    0.4723
    0.6965    0.4960    0.0590         0    0.3835    0.4723    0.4723
    0.6965    0.4960    0.3835    0.3835         0    0.3750    0.3750
    0.7960    0.6730    0.4723    0.4723    0.3750         0    0.3750
    0.7960    0.6730    0.4723    0.4723    0.3750    0.3750         0
    0.8355    0.7080    0.5714    0.5714    0.4275    0.4275    0.2960
    0.8355    0.7080    0.5714    0.5714    0.5714    0.5714    0.3710
    0.9090    0.7227    0.7227    0.7227    0.5714    0.5714    0.4380
  Columns 8 through 10

    0.8355    0.8355    0.9090
    0.7080    0.7080    0.7227
    0.5714    0.5714    0.7227
    0.5714    0.5714    0.7227
    0.4275    0.5714    0.5714
    0.4275    0.5714    0.5714
    0.2960    0.3710    0.4380
         0    0.3710    0.4380
    0.3710         0    0.4000
    0.4380    0.4000         0


vaf =

    0.7210


outperm =

     1     2     3     5     4     6     7    10     9     8
```

9.4 The Use of Optimal Transformations and the m-function proxmon.m

As previously discussed within Part I, the MATLAB function, `proxmon.m`, provides a monotonically transformed proximity matrix that is close in a least-squares sense to a given input matrix. The syntax is

```
[monproxpermut vaf diff] = proxmon(proxpermut,fitted)
```

where `PROXPERMUT` is the input proximity matrix (which may have been subjected to an initial row/column permutation, hence the suffix '`PERMUT`') and `FITTED` is a given target matrix; the output matrix `MONPROXPERMUT` is closest to `FITTED` in a least-squares sense and obeys the order constraints obtained from each pair of entries in (the upper-triangular portion of) `PROXPERMUT` (and where the inequality constrained optimization is carried out using the Dykstra-Kaczmarz iterative projection strategy); `VAF` denotes 'variance-accounted-for' and indicates how much variance in `MONPROXPERMUT` can be accounted for by `FITTED`; finally `DIFF` is the value of the least-squares loss function and is (one-half) the sum of squared differences between the entries in `MONPROXPERMUT` and `FITTED`.

In the notation of the introduction when fitting a given order, `FITTED` would correspond to the AR matrix $\mathbf{A} = \{a_{ij}\}$; the input `PROXPERMUT` would be $\{p_{\rho^0(i)\rho^0(j)}\}$; `MONPROXPERMUT` would be $\{f(p_{\rho^0(i)\rho^0(j)})\}$, where the function $f(\cdot)$ satisfies the monotonicity constraints, i.e., if $p_{\rho^0(i)\rho^0(j)} < p_{\rho^0(i')\rho^0(j')}$ for $1 \leq i < j \leq n$ and $1 \leq i' < j' \leq n$, then $f(p_{\rho^0(i)\rho^0(j)}) \leq f(p_{\rho^0(i')\rho^0(j')})$. The transformed proximity matrix $\{f(p_{\rho^0(i)\rho^0(j)})\}$ minimizes the least-squares criterion (`DIFF`) of

$$\sum_{i<j}(f(p_{\rho^0(i)\rho^0(j)}) - a_{ij})^2,$$

over all functions $f(\cdot)$ that satisfy the monotonicity constraints. The `VAF` is a normalization of this loss value by the sum of squared deviations of the transformed proximities from their mean:

$$\text{VAF} = 1 - \frac{\sum_{i<j}(f(p_{\rho^0(i)\rho^0(j)}) - a_{ij})^2}{\sum_{i<j}(f(p_{\rho^0(i)\rho^0(j)}) - \bar{f})^2},$$

where $\bar{f}$ denotes the mean of the off-diagonal entries in $\{f(p_{\rho^0(i)\rho^0(j)})\}$.

The script m-file listed below gives an application of `proxmon.m` along with finding a best fitting AR form for our `number.dat` matrix. First, `arobfnd.m` is invoked to obtain a best-fitting AR matrix (`fit`); this is the same as found before based on the `outperm` of [1 2 3 5 4 6 7 9 10 8] with a `vaf` of .7782. The m-file, `proxmon.m`, is then used to generate the monotonically transformed proximity matrix (`monproxpermut`) with `vaf` of .8323. Given the SIOT (single-iteration-optimal-transformation) discussion of the introduction, it might now be best to fit once more an AR matrix to this now monotonically transformed proximity matrix, but then stop. Otherwise as seen in the output below, if the strategy is repeated cyclically (i.e., finding a fitted matrix based on the monotonically transformed proximity matrix, finding a new monotonically transformed matrix, and so on), a perfect `vaf` of 1.0 can be achieved at the expense of losing most of the detail in the transformed proximities, i.e., only five distinct values remain that correspond to the three largest and single smallest of the original proximities with *all* the remaining now tied at a value of .5467. (To avoid another type of degeneracy (where all matrices would converge to zeros), the sum of squares of the fitted matrix is kept the same as it was initially; convergence is based on observing a minimal change (less than 1.0e-010) in the `vaf`.

```
load number.dat
[fit vaf outperm] = arobfnd(number,randperm(10),2)
[monproxpermut vaf diff] = ...
    proxmon(number(outperm,outperm),fit)
sumfitsq = sum(sum(fit.^2));
prevvaf = 2;
while (abs(prevvaf-vaf) >= 1.0e-010)
   prevvaf = vaf;
   [fit vaf] = arobfit(monproxpermut,1:10);
   sumnewfitsq = sum(sum(fit.^2));
   fit = sqrt(sumfitsq)*(fit/sqrt(sumnewfitsq));
```

```
    [monproxpermut vaf diff] = proxmon(number(outperm,outperm), fit);
end

outperm
fit


monproxpermut
number(outperm,outperm)
vaf
diff

fit =

  Columns 1 through 7

         0    0.4210    0.5840    0.6840    0.7090    0.7960    0.7960
    0.4210         0    0.2840    0.4960    0.4960    0.5880    0.7357
    0.5840    0.2840         0    0.0590    0.3835    0.4928    0.4928
    0.6840    0.4960    0.0590         0    0.3835    0.3985    0.3985
    0.7090    0.4960    0.3835    0.3835         0    0.3750    0.3750
    0.7960    0.5880    0.4928    0.3985    0.3750         0    0.3750
    0.7960    0.7357    0.4928    0.3985    0.3750    0.3750         0
    0.8210    0.7357    0.4928    0.4928    0.4928    0.4928    0.3460
    0.8500    0.7357    0.7357    0.6830    0.4928    0.4928    0.3460
    0.9090    0.7357    0.7357    0.7357    0.5920    0.4928    0.4253

  Columns 8 through 10

    0.8210    0.8500    0.9090
    0.7357    0.7357    0.7357
    0.4928    0.7357    0.7357
    0.4928    0.6830    0.7357
    0.4928    0.4928    0.5920
    0.4928    0.4928    0.4928
    0.3460    0.3460    0.4253
         0    0.3460    0.4253
    0.3460         0    0.4253
    0.4253    0.4253         0


vaf =
    0.7782


outperm =

     1     2     3     5     4     6     7     9    10     8


monproxpermut =

  Columns 1 through 7

         0    0.4244    0.5549    0.6840    0.7058    0.7659    0.7058
    0.4244         0    0.3981    0.5908    0.4054    0.5549    0.7058
    0.5549    0.3981         0    0.0590    0.4054    0.5908    0.4310
    0.6840    0.5908    0.0590         0    0.4244    0.4244    0.4054
    0.7058    0.4054    0.4054    0.4244         0    0.4310    0.3981
    0.7659    0.5549    0.5908    0.4244    0.4310         0    0.4054
    0.7058    0.7058    0.4310    0.4054    0.3981    0.4054         0
    0.8210    0.7058    0.4054    0.3981    0.7058    0.5908    0.4054
    0.8500    0.5908    0.7659    0.6830    0.3981    0.5549    0.3981
    0.9090    0.5908    0.7058    0.7058    0.5908    0.4244    0.4244

  Columns 8 through 10

    0.8210    0.8500    0.9090
    0.7058    0.5908    0.5908
    0.4054    0.7659    0.7058
    0.3981    0.6830    0.7058
    0.7058    0.3981    0.5908
    0.5908    0.5549    0.4244
    0.4054    0.3981    0.4244
         0    0.4054    0.4244
    0.4054         0    0.4310
    0.4244    0.4310         0


vaf =

    0.8323
```

```
diff =

    0.2075


outperm =

     1     2     3     5     4     6     7     9    10     8


fit =

  Columns 1 through 7

         0    0.5467    0.5467    0.5467    0.5467    0.5467    0.5467
    0.5467         0    0.5467    0.5467    0.5467    0.5467    0.5467
    0.5467    0.5467         0    0.0609    0.5467    0.5467    0.5467
    0.5467    0.5467    0.0609         0    0.5467    0.5467    0.5467
    0.5467    0.5467    0.5467    0.5467         0    0.5467    0.5467
    0.5467    0.5467    0.5467    0.5467    0.5467         0    0.5467
    0.5467    0.5467    0.5467    0.5467    0.5467    0.5467         0
    0.8474    0.5467    0.5467    0.5467    0.5467    0.5467    0.5467
    0.8774    0.5467    0.5467    0.5467    0.5467    0.5467    0.5467
    0.9383    0.5467    0.5467    0.5467    0.5467    0.5467    0.5467

  Columns 8 through 10

    0.8474    0.8774    0.9383
    0.5467    0.5467    0.5467
    0.5467    0.5467    0.5467
    0.5467    0.5467    0.5467
    0.5467    0.5467    0.5467
    0.5467    0.5467    0.5467
    0.5467    0.5467    0.5467
         0    0.5467    0.5467
    0.5467         0    0.5467
    0.5467    0.5467         0


monproxpermut =

  Columns 1 through 7
```

```
         0    0.5467    0.5467    0.5467    0.5467    0.5467    0.5467
    0.5467         0    0.5467    0.5467    0.5467    0.5467    0.5467
    0.5467    0.5467         0    0.0609    0.5467    0.5467    0.5467
    0.5467    0.5467    0.0609         0    0.5467    0.5467    0.5467
    0.5467    0.5467    0.5467    0.5467         0    0.5467    0.5467
    0.5467    0.5467    0.5467    0.5467    0.5467         0    0.5467
    0.5467    0.5467    0.5467    0.5467    0.5467    0.5467         0
    0.8474    0.5467    0.5467    0.5467    0.5467    0.5467    0.5467
    0.8774    0.5467    0.5467    0.5467    0.5467    0.5467    0.5467
    0.9383    0.5467    0.5467    0.5467    0.5467    0.5467    0.5467

  Columns 8 through 10

    0.8474    0.8774    0.9383
    0.5467    0.5467    0.5467
    0.5467    0.5467    0.5467
    0.5467    0.5467    0.5467
    0.5467    0.5467    0.5467
    0.5467    0.5467    0.5467
    0.5467    0.5467    0.5467
         0    0.5467    0.5467
    0.5467         0    0.5467
    0.5467    0.5467         0


ans =

  Columns 1 through 7

         0    0.4210    0.5840    0.6840    0.7090    0.8040    0.7880
    0.4210         0    0.2840    0.6460    0.3460    0.5880    0.7580
    0.5840    0.2840         0    0.0590    0.3540    0.6710    0.4210
    0.6840    0.6460    0.0590         0    0.4130    0.4090    0.3880
    0.7090    0.3460    0.3540    0.4130         0    0.4290    0.3000
    0.8040    0.5880    0.6710    0.4090    0.4290         0    0.3960
    0.7880    0.7580    0.4210    0.3880    0.3000    0.3960         0
    0.8210    0.7910    0.3670    0.2460    0.8040    0.6710    0.3500
    0.8500    0.6250    0.8080    0.6830    0.2630    0.5920    0.2960
    0.9090    0.6300    0.7960    0.7420    0.5920    0.4000    0.4170

  Columns 8 through 10
```

```
    0.8210    0.8500    0.9090
    0.7910    0.6250    0.6300
    0.3670    0.8080    0.7960
    0.2460    0.6830    0.7420
    0.8040    0.2630    0.5920
    0.6710    0.5920    0.4000
    0.3500    0.2960    0.4170
         0    0.3920    0.4000
    0.3920         0    0.4590
    0.4000    0.4590         0


vaf =

    1.0000


diff =

  8.3999e-011
```

9.5 Representing SAR Structures (Graphically)

The use of the very general form of representation offered by an AR matrix without the imposition of any further restrictions has one annoying interpretive difficulty. Specifically, it is usually necessary to interpret the fitted structures directly (and enumeratively) through a set of subsets or clusters that are all defined by objects contiguous in a specific object ordering; each such subset has an attached diameter that reflects its maximum within-class fitted value. More pointedly, it is generally *not* possible to use a more convenient graph-theoretic structure and the lengths of paths between objects in such a graph to represent visually a fitted AR matrix; this situation contrasts with opportunities resulting when the approximation matrix is more restricted and defined, say, by an ultrametric or an additive tree, or by a (linear or circular) unidimensional scaling (see Hubert, Arabie, & Meulman, 1997).

As noted in the introduction, the imposition of SAR conditions permits a representation of the fitted values in a (least-squares) SAR approximating matrix as lengths of paths in a graph, although this graph will not generally have the simplified form of a tree. A discussion of these latter SAR constraints is not new here, and a number of (theoretical) presentations of their usefulness exist in the literature (for example, see Critchley and Fichet, 1994; Critchley, 1994; Durand and Fichet, 1988; Mirkin, 1996, Chapter 7). Here, we give the example based on the number data from Hubert, Arabie, and Meulman (1998) for interpretative

Table 9.1: Order-constrained least-squares approximations to the digit proximity data of Shepard *et al.* (1975); the upper-triangular portion is anti-Robinson and the lower-triangular portion is strongly-anti-Robinson

digit	0	1	2	4	3	5	6	8	9	7
0	x	3.41	4.21	4.70	4.83	5.25	5.25	5.38	5.52	5.81
1	3.41	x	2.73	3.78	3.78	4.23	4.96	4.96	4.96	4.96
2	4.21	2.73	x	1.63	3.22	3.76	3.76	3.76	4.96	4.96
4	4.76	3.78	1.63	x	3.22	3.30	3.30	3.76	4.70	4.96
3	4.76	3.78	3.22	3.22	x	3.18	3.18	3.76	3.76	4.25
5	5.25	4.59	3.53	3.53	3.18	x	3.18	3.76	3.76	3.76
6	5.25	4.59	3.53	3.53	3.18	3.18	x	3.04	3.04	3.43
8	5.57	4.96	4.18	4.18	4.18	4.18	3.04	x	3.04	3.43
9	5.57	4.96	4.18	4.18	4.18	4.18	3.04	3.04	x	3.43
7	5.57	4.96	4.18	4.18	4.18	4.18	3.43	3.43	3.43	x

convenience. The latter data were transformed (in that reference) to a standard deviation of 1.0 and a mean of 4.0; thus, the numbers within the fitted matrices will differ from the examples given earlier. Approximating AR and SAR forms for the transformed number proximity data are given in the upper and lower-triangular portions, respectively, of the matrix in Table 9.1. For convenience below, we will denote the upper-triangular AR matrix by $\mathbf{A}_{ut}$ and the lower-triangular SAR matrix by $\mathbf{A}_{lt}$.

The $10(10-1)/2 = 45$ subsets defined by objects contiguous in the object ordering used to display the upper-triangular portion of Table 9.1 are listed in Table 9.2 according to increasing diameter values. For purposes of our later discussion, 22 of the subsets are given in italics to indicate that they are proper subsets of another listed subset having the same diameter. Substantively, the dominant patterning of the entries in $\mathbf{A}_{ut}$ appears to reflect (primarily) digit magnitude except for the placement of digit 4 next to 2, and digit 7 being located in the last position. Both these latter deviations from an interpretation strictly according to digit magnitude show some of the salient structural properties of the digits. For example, the digit pair (2,4) has the absolute smallest dissimilarity in the data; besides being relatively close in magnitude, there are the possible (although redundant) similarity bases that $2 + 2 = 4$, $2 \times 2 = 4$, 4 is a power of 2, and both 2 and 4 are even numbers. Similarly, the placement of the digit 7 in the last position results from the salience of the triple $\{6, 8, 9\}$, which is the third to emerge according to its diameter. In addition to these three digits all being relatively close in magnitude, 6 and 8 are both even numbers, 6 and 9 are multiples of 3, and 8 is directly adjacent in size to 9. The three original dissimilarities within the set $\{6, 8, 9\}$ are all smaller than the dissimilarities digit 7 has to *any* other digit.

Given just the collection of subsets $S_1, \ldots, S_M$ listed in Table 9.2 and their associated diameters, it is possible (trivially) to reconstruct the original approximating matrix $\mathbf{A}_{ut}$ by

Table 9.2: The 45 subsets listed according to increasing diameter values that are contiguous in the object ordering used to display the upper-triangular portion of Table 9.1. The 22 subsets given in italics are redundant in the sense that they are proper subsets of another listed subset with the same diameter.

subset	*diameter*
{2,4}	1.63
{1,2}	2.73
{*6,8*},{*8,9*},{6,8,9}	3.04
{*3,5*},{*5,6*},{3,5,6}	3.18
{*4,3*},{2,4,3}	3.22
{*4,3,5*},{4,3,5,6}	3.30
{0,1}	3.41
{*9,7*},{*8,9,7*},{6,8,9,7}	3.43
{*5,6,8*},{*5,6,8,9*},{5,6,8,9,7}	3.76
{*3,5,6,8*},{3,5,6,8,9}	3.76
{*4,3,5,6,8*},{*2,4,3,5*},{*2,4,3,5,6*},{2,4,3,5,6,8}	3.76
{*1,2,4*},{1,2,4,3}	3.78
{0,1,2}	4.21
{1,2,4,3,5}	4.23
{3,5,6,8,9,7}	4.25
{0,1,2,4},{4,3,5,6,8,9}	4.70
{0,1,2,4,3}	4.83
{*1,2,4,3,5,6*},{*1,2,4,3,5,6,8*}	4.96
{*1,2,4,3,5,6,8,9*},{*2,4,3,5,6,8,9*}	4.96
{*2,4,3,5,6,8,9,7*},{*4,3,5,6,8,9,7*}	4.96
{1,2,4,3,5,6,8,9,7}	4.96
{*0,1,2,4,3,5*},{0,1,2,4,3,5,6}	5.25
{0,1,2,4,3,5,6,8}	5.38
{0,1,2,4,3,5,6,8,9}	5.52
{0,1,2,4,3,5,6,8,9,7}	5.81

identifying for each object pair the smallest diameter for a subset that contains that pair. (Explicitly, the smallest diameter for a subset that contains an object pair is equal to the value in $\mathbf{A}_{ut}$ associated with that pair, and the subset itself includes that object pair and all objects in between in the ordering that is used to display the AR form for $\mathbf{A}_{ut}$.) This type of reconstruction is generally possible for any matrix that can be row/column reordered to an AR form through the collection of subsets $S_1, \ldots, S_M$ and their diameters identified by increasing a threshold variable from the smallest fitted value. In fact, even if all the italicized subsets were removed (that are proper subsets of another having the same diameter), exactly the same reconstruction could be carried out because the italicized subsets are redundant with respect to identifying for each object pair the smallest diameter for a subset that contains the pair.

Without imposing further restrictions on the approximating matrix other than just being AR, a more convenient representation using a graph and path lengths in such a graph is generally not possible. We will select two small (AR) submatrices from the upper-triangular portion of Table 9.1 to make this point more convincingly, and in the process indicate by example how a graph representation is to be constructed and why further restrictions on the approximating matrix may be necessary to carry out the task.

First, consider the fitted values for the first four placed digits, 0, 1, 2, and 4, for which the desired type of graphical representation *is* possible without imposing any further constraints. This AR submatrix is given in Figure 9.1(a) along with the six corresponding subsets of contiguous objects and their diameters, and a graphical representation for the structure. The latter consists of four nodes corresponding to the original four objects that we represent by open circles (referred to as "terminal" nodes), plus six nodes represented by solid circles that denote the six subsets in the given listing (referred to as "internal nodes"). Based on this graph and the internal node heights provided by the calibrated scale on the left, a fitted value in the submatrix between any two terminal nodes can be obtained as one-half the length of the minimum path from one of the terminal nodes up to an internal node and back down to the other terminal node. All horizontal line segments are used here for display convenience only and are assumed not to contribute to the length of any path. Thus, if we changed the vertical scaling by a multiplier of 1/2, each of the fitted values in the submatrix would be exactly the length of the minimum path, between two terminal nodes, that proceeded upward from one such node to an internal node and then back down to the other. We might also note that from the topmost internal node, all paths down to the terminal nodes have exactly the same length; i.e., there is an internal node equidistant from all terminal nodes.

Now, consider the fitted values for the four objects placed respectively at the third through sixth positions: 2, 4, 3, and 5. This AR submatrix is given in Figure 9.1(b) along with the corresponding subsets of contiguous objects and their diameters (excluding the redundant subset {4,3} which is a proper subset of {2,4,3} having the same diameter), and the beginnings of a graphical representation for its structure. There is a difficulty encountered, however, in defining a graph that would be completely consistent with all the fitted values in the 4×4 submatrix; we indicate this anomaly by the dashed vertical and horizontal lines. If an internal node were to be placed at the level of 3.30 to represent the cluster $\{4, 3, 5\}$,

Table 9.3: The fourteen (nonredundant) subsets listed according to increasing diameter values are contiguous in the linear object ordering used to display the lower-triangular SAR portion of Table 9.1.

subset	*diameter*	*subset*	*diameter*
{2,4}	1.63	{2,4,3,5,6}	3.53
{1,2}	2.73	{1,2,4,3}	3.78
{6,8,9}	3.04	{2,4,3,5,6,8,9,7}	4.18
{3,5,6}	3.18	{0,1,2}	4.21
{2,4,3}	3.22	{0,1,2,4,3}	4.76
{0,1}	3.41	{0,1,2,4,3,5,6}	5.25
{6,8,9,7}	3.43	{0,1,2,4,3,5,6,8,9,7}	5.57

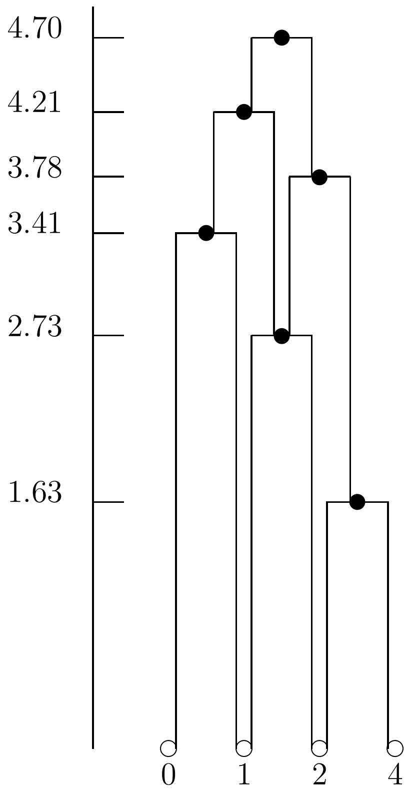
by implication the fitted value for the digit pair (2,5) should also be 3.30 (and not its current value of 3.76). Because digit 3 was "joined" to *both* 2 and 4 at the threshold level 3.22, and thus, there are two fitted values tied at 3.22, a consistent graphical representation would be possible only if the fitted values for the pairs (2,5) and (4,5) were equal. This last observation, that when some fitted values are tied in an approximating matrix $\mathbf{A}_{ut}$, others must also be tied to allow for the construction of a consistent graphical representation, is the motivating basis for considering an additional set of SAR constraints.

When a graphical representation that permits their reconstruction through path lengths is desired for the collection of fitted values in an approximating matrix $\mathbf{A}$, the small illustration just provided serves as justification for imposing a stricter collection of constraints on the approximating matrix than just being row/column reorderable to an AR form. In particular, the additional restriction will be imposed that the approximating matrix $\mathbf{A}$ is row/column reorderable to one that is SAR, which will eliminate the type of graphical anomaly present in Figure 9.1(b).

For the SAR approximation given in the lower-triangular portion of Table 9.1, there are now only fourteen (nonredundant) subsets identifiable by increasing a threshold variable from the smallest fitted value; these are listed in Table 9.3 along with their diameters. The imposition of the more restrictive SAR constraints allows the graphical representation given in Figure 9.2. Although we might not change our substantive comments about the approximating matrix (i.e., mostly digit magnitude with some structural characteristics for the subsets $\{2,4\}$ and $\{6,8,9\}$), a graphical representation makes these same observations visually clearer.

(a)

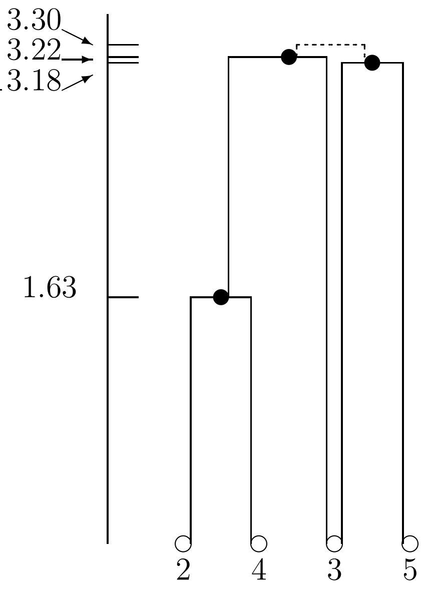
	0	1	2	4
0	x	3.41	4.21	4.70
1		x	2.73	3.78
2			x	1.63
4				x



subset	*diameter*
{2,4}	1.63
{1,2}	2.73
{0,1}	3.41
{1,2,4}	3.78
{0,1,2}	4.21
{0,1,2,4}	4.70

(b)

	2	4	3	5
2	x	1.63	3.22	3.76
4		x	3.22	3.30
3			x	3.18
5				x



subset	*diameter*
{2,4}	1.63
{3,5}	3.18
{2,4,3}	3.22
{4,3,5}	3.30
{2,4,3,5}	3.76

Figure 9.1: Two 4 × 4 submatrices and the object subsets they induce, taken from the anti-Robinson matrix in the upper-triangular portion of Table 9.1. For (a), a graphical representation of the fitted values is possible; for (b), the anomaly indicated by the dashed lines prevents a consistent graphical representation from being constructed.

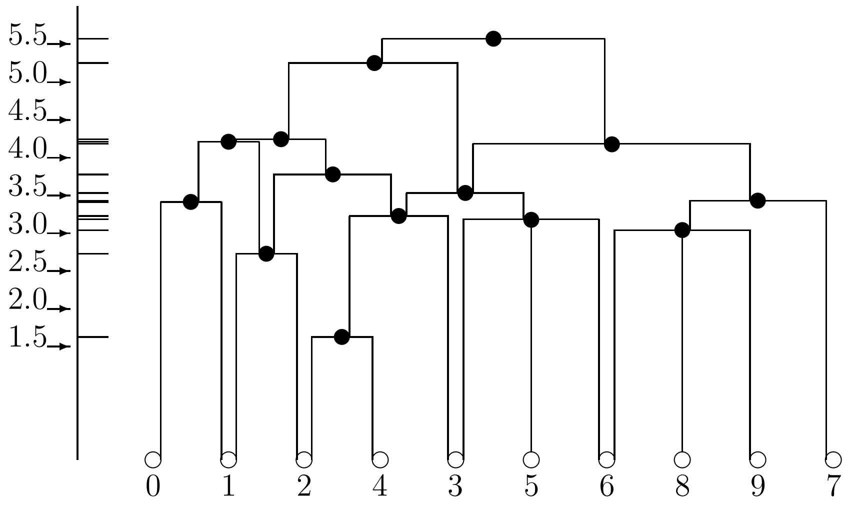


Figure 9.2: A graphical representation for the fitted values given by the strongly-anti-Robinson matrix in the lower-triangular portion of Table 9.1.

9.6 Representation Through Multiple (Strongly) AR Matrices

The representation of a proximity matrix by a single anti-Robinson structure extends easily to the additive use of multiple matrices. The m-function, `biarobfnd.m`, fits the sum of two anti-Robinson matrices using iterative projection to a symmetric proximity matrix in the L_2-norm based on permutations identified through the use of iterative quadratic assignment. The usage syntax is

```
[find,vaf,targone,targtwo,outpermone,outpermtwo] = ...
biarobfnd(prox,inperm,kblock)
```

where, as before, `PROX` is the input proximity matrix ($n \times n$ with a zero main diagonal and a dissimilarity interpretation); `INPERM` is a given starting permutation of the first n integers; `FIND` is the least-squares optimal matrix (with variance-accounted-for of `VAF`) to `PROX` and is the sum of the two anti-Robinson matrices `TARGONE` and `TARGTWO` based on the two row and column object orderings given by the ending permutations `OUTPERMONE` and `OUTPERMTWO`. As before, `KBLOCK` defines the block size in the use the iterative quadratic assignment routine.

In the example below, the two resulting AR forms are very clearly interpretable as number magnitude and digit structural properties; the variance-accounted-for is, in effect, 100%.

```
load number.dat
[find,vaf,targone,targtwo,outpermone,outpermtwo] = ...
biarobfnd(number,1:10,1)
```

```
find =

  Columns 1 through 7

         0    0.4209    0.5840    0.7090    0.6840    0.8040    0.7865
    0.4209         0    0.2840    0.3460    0.6460    0.5880    0.7568
    0.5840    0.2840         0    0.3540    0.0588    0.6702    0.4225
    0.7090    0.3460    0.3540         0    0.4130    0.4290    0.3000
    0.6840    0.6460    0.0588    0.4130         0    0.4094    0.3880
    0.8040    0.5880    0.6702    0.4290    0.4094         0    0.3960
    0.7865    0.7568    0.4225    0.3000    0.3880    0.3960         0
    0.9107    0.6300    0.7960    0.5920    0.7420    0.4000    0.4169
    0.8210    0.7975    0.3672    0.7975    0.2460    0.6714    0.3499
    0.8500    0.6250    0.8080    0.2630    0.6829    0.5920    0.2960

  Columns 8 through 10

    0.9107    0.8210    0.8500
    0.6300    0.7975    0.6250
    0.7960    0.3672    0.8080
    0.5920    0.7975    0.2630
    0.7420    0.2460    0.6829
    0.4000    0.6714    0.5920
    0.4169    0.3499    0.2960
         0    0.4000    0.4587
    0.4000         0    0.3922
    0.4587    0.3922         0


vaf =

    0.9999


targone =

  Columns 1 through 7

         0    0.3406    0.6710    0.6926    0.6956    0.6956    0.8303
    0.3406         0    0.2018    0.5421    0.5423    0.5880    0.6764
    0.6710    0.2018         0    0.3333    0.3680    0.4662    0.4662
    0.6926    0.5421    0.3333         0    0.3093    0.3206    0.3779
    0.6956    0.5423    0.3680    0.3093         0    0.2055    0.3779
    0.6956    0.5880    0.4662    0.3206    0.2055         0    0.2876
    0.8303    0.6764    0.4662    0.3779    0.3779    0.2876         0
    0.8303    0.6764    0.6764    0.6764    0.6383    0.4675    0.3360
    0.8303    0.7511    0.7138    0.6764    0.6383    0.4745    0.3366
    0.8611    0.7943    0.7943    0.6764    0.6690    0.4836    0.3849

  Columns 8 through 10

    0.8303    0.8303    0.8611
    0.6764    0.7511    0.7943
    0.6764    0.7138    0.7943
    0.6764    0.6764    0.6764
    0.6383    0.6383    0.6690
    0.4675    0.4745    0.4836
    0.3360    0.3366    0.3849
         0    0.2243    0.3783
    0.2243         0    0.3783
    0.3783    0.3783         0


targtwo =

  Columns 1 through 7

         0   -0.3923   -0.3092   -0.0093    0.0139    0.0139    0.1211
   -0.3923         0   -0.3092   -0.0116    0.0101    0.0139    0.1037
   -0.3092   -0.3092         0   -0.0870   -0.0438    0.0137    0.0207
   -0.0093   -0.0116   -0.0870         0   -0.0438   -0.0111    0.0164
    0.0139    0.0101   -0.0438   -0.0438         0   -0.0889   -0.0779
    0.0139    0.0139    0.0137   -0.0111   -0.0889         0   -0.4134
    0.1211    0.1037    0.0207    0.0164   -0.0779   -0.4134         0
    0.1211    0.1037    0.0822    0.0804    0.0804   -0.1693   -0.1961
    0.1757    0.1037    0.0822    0.0804    0.0804    0.0804   -0.0844
    0.2039    0.2039    0.2039    0.1084    0.1084    0.1084    0.1084

  Columns 8 through 10

    0.1211    0.1757    0.2039
    0.1037    0.1037    0.2039
    0.0822    0.0822    0.2039
    0.0804    0.0804    0.1084
    0.0804    0.0804    0.1084
   -0.1693    0.0804    0.1084
   -0.1961   -0.0844    0.1084
         0   -0.1211         0
   -0.1211         0   -0.0745
         0   -0.0745         0


outpermone =

     1     2     3     4     5     6     7     9     8    10


outpermtwo =

     9     5     3     1     7    10     4     2     8     6
```

For finding multiple SAR forms, `bisarobfnd.m` has usage syntax

`[find,vaf,targone,targtwo,outpermone,outpermtwo] = bisarobfnd(prox,inperm,kblock)`

with all the various terms the same as for `biarobfnd.m` but now for strongly AR (SAR) structures. The example below finds essentially the same representation as above (involving digit magnitude and structure) with a slight drop in the variance-accounted-for of 99.06%.

```
[find,vaf,targone,targtwo,outpermone,outpermtwo] = bisarobfnd(number,randperm(10),1)

find =

  Columns 1 through 7

         0    0.4210    0.5840    0.7095    0.6838    0.8519    0.7260
    0.4210         0    0.2840    0.3460    0.6461    0.5892    0.7565
    0.5840    0.2840         0    0.3541    0.0590    0.6090    0.4830
    0.7095    0.3460    0.3541         0    0.4131    0.4278    0.3005
    0.6838    0.6461    0.0590    0.4131         0    0.4090    0.3882
    0.8519    0.5892    0.6090    0.4278    0.4090         0    0.3960
    0.7260    0.7565    0.4830    0.3005    0.3882    0.3960         0
    0.8998    0.6153    0.8059    0.6067    0.7286    0.4000    0.4168
    0.8208    0.8246    0.3670    0.7893    0.2460    0.6711    0.3502
    0.8736    0.6250    0.7797    0.2630    0.6965    0.5920    0.2955

  Columns 8 through 10
```

```
    0.8998    0.8208    0.8736
    0.6153    0.8246    0.6250
    0.8059    0.3670    0.7797
    0.6067    0.7893    0.2630
    0.7286    0.2460    0.6965
    0.4000    0.6711    0.5920
    0.4168    0.3502    0.2955
         0    0.4000    0.4590
    0.4000         0    0.3921
    0.4590    0.3921         0


vaf =

    0.9906


targone =

  Columns 1 through 7

         0    0.3148    0.6038    0.6296    0.6296    0.7457    0.7457
    0.3148         0    0.1778    0.5201    0.5201    0.6626    0.6626
    0.6038    0.1778         0    0.2742    0.3230    0.5028    0.5028
    0.6296    0.5201    0.2742         0    0.3192    0.5012    0.5012
    0.6296    0.5201    0.3230    0.3192         0    0.2831    0.3340
    0.7457    0.6626    0.5028    0.5012    0.2831         0    0.3021
    0.7457    0.6626    0.5028    0.5012    0.3340    0.3021         0
    0.7936    0.7061    0.6997    0.6974    0.6027    0.5526    0.3229
    0.7936    0.7061    0.6997    0.6974    0.6027    0.5526    0.3229
    0.7936    0.7061    0.6997    0.6974    0.6027    0.5527    0.4963

  Columns 8 through 10

    0.7936    0.7936    0.7936
    0.7061    0.7061    0.7061
    0.6997    0.6997    0.6997
    0.6974    0.6974    0.6974
    0.6027    0.6027    0.6027
    0.5526    0.5526    0.5527
    0.3229    0.3229    0.4963
         0    0.2815    0.4197
    0.2815         0    0.3001
    0.4197    0.3001         0


targtwo =

  Columns 1 through 7

         0   -0.3567   -0.2640    0.0542    0.0542    0.0938    0.0938
   -0.3567         0   -0.3327    0.0272    0.0272    0.0919    0.0919
   -0.2640   -0.3327         0   -0.0198   -0.0198    0.0799    0.0799
    0.0542    0.0272   -0.0198         0   -0.0198    0.0799    0.0799
    0.0542    0.0272   -0.0198   -0.0198         0   -0.2008   -0.2008
    0.0938    0.0919    0.0799    0.0799   -0.2008         0   -0.4344
    0.0938    0.0919    0.0799    0.0799   -0.2008   -0.4344         0
    0.1260    0.1185    0.1062    0.1062    0.0939   -0.0811   -0.1741
    0.1260    0.1185    0.1062    0.1062    0.0939    0.0393   -0.0907
    0.1260    0.1185    0.1062    0.1062    0.0939    0.0393   -0.0734

  Columns 8 through 10

    0.1260    0.1260    0.1260
    0.1185    0.1185    0.1185
    0.1062    0.1062    0.1062
    0.1062    0.1062    0.1062
    0.0939    0.0939    0.0939
   -0.0811    0.0393    0.0393
   -0.1741   -0.0907   -0.0734
         0   -0.0907   -0.0734
   -0.0907         0   -0.1526
   -0.0734   -0.1526         0


outpermone =

     1     2     3     4     5     6     7     8     9    10


outpermtwo =

     5     9     3     1     7    10     4     2     8     6
```

Chapter 10

Circular-Anti-Robinson (CAR) Matrices for Symmetric Proximity Data

In the approximation of a proximity matrix $\mathbf{P}$ by one that is row/column reorderable to an AR form, the interpretation of the fitted matrix in general had to be carried out by identifying a set of subsets through an increasing threshold variable; each of the subsets contained objects that were contiguous with respect to a given *linear* ordering along a continuum, and had a diameter defined by the maximum fitted value within the subset. To provide a further representation depicting the fitted values as lengths of paths in a graph, an approximation was sought that satisfied the additional constraints of an SAR matrix; still, the subsets thus identified had to contain objects contiguous with respect to a linear ordering. As one possible generalization of both the AR and SAR constraints, we can define what will be called circular anti-Robinson (CAR) and circular strongly-anti-Robinson (CSAR) forms that allow the subsets identified from increasing a threshold variable to be contiguous with respect to a *circular* ordering of the objects around a closed continuum. Approximation matrices that are row/column reorderable to display an AR or SAR form respectively will also be (trivially) row/column reorderable to display what is formally characterized below as a CAR or a CSAR form, but not conversely. (Historically, there is a large literature on the possibility of circular structures emerging from and being identifiable in a given proximity matrix, with the CAR concept discussed most extensively under the term "circumplex". One of the earliest references is to Guttman [1954], but for a variety of others the reader is referred to the discussion of metric circular unidimensional scaling in Hubert, Arabie, and Meulman [1997]. The extension of CAR forms to those that are also CSAR, however, has apparently not been a topic discussed in the literature before the appearance of Hubert, Arabie, and Meulman [1998]; this latter source forms the basis for much of the present chapter.)

To be explicit, an arbitrary symmetric matrix $\mathbf{Q} = \{q_{ij}\}$, where $q_{ii} = 0$ for $1 \leq i, j \leq n$, is said to be row/column reorderable to a circular anti-Robinson form (or, for short, $\mathbf{Q}$ is a circular anti-Robinson (CAR) matrix) if there exists a permutation, $\rho(\cdot)$, on the first n

integers such that the reordered matrix $\mathbf{Q}_\rho = \{q_{\rho(i)\rho(j)}\}$ satisfies the conditions given in (II):

(II): for $1 \leq i \leq n-3$, and $i+1 < j \leq n-1$,

if $q_{\rho(i+1)\rho(j)} \leq q_{\rho(i)\rho(j+1)}$, then
$q_{\rho(i+1)\rho(j)} \leq q_{\rho(i)\rho(j)}$ and $q_{\rho(i+1)\rho(j)} \leq q_{\rho(i+1)\rho(j+1)}$;
if $q_{\rho(i+1)\rho(j)} \geq q_{\rho(i)\rho(j+1)}$, then
$q_{\rho(i)\rho(j)} \geq q_{\rho(i)\rho(j+1)}$ and $q_{\rho(i+1)\rho(j+1)} \geq q_{\rho(i)\rho(j+1)}$,
and, for $2 \leq i \leq n-2$,
if $q_{\rho(i+1)\rho(n)} \leq q_{\rho(i)\rho(1)}$, then
$q_{\rho(i+1)\rho(n)} \leq q_{\rho(i)\rho(n)}$ and $q_{\rho(i+1)\rho(n)} \leq q_{\rho(i+1)\rho(1)}$;
if $q_{\rho(i+1)\rho(n)} \geq q_{\rho(i)\rho(1)}$, then
$q_{\rho(i)\rho(n)} \geq q_{\rho(i)\rho(1)}$ and $q_{\rho(i+1)\rho(1)} \geq q_{\rho(i)\rho(1)}$.

Interpretatively, within each row of $\mathbf{Q}_\rho$ moving to the right from the main diagonal and then wrapping back around to re-enter the same row from the left, the entries never decrease until a maximum is reached and then never increase moving away from the maximum until the main diagonal is again reached. Given the symmetry of $\mathbf{P}$, a similar pattern of entries would be present within each column as well. As noted above, any AR matrix is CAR but not conversely.

In analogy to the SAR conditions that permit graphical representation, a symmetric matrix $\mathbf{Q}$ is said to be row/column reorderable to a circular strongly-anti-Robinson form (or, for short, $\mathbf{Q}$ is a circular strongly-anti-Robinson (CSAR) matrix) if there exists a permutation, $\rho(\cdot)$, on the first n integers such that the reordered matrix $\mathbf{Q}_\rho = \{q_{\rho(i)\rho(j)}\}$ satisfies the conditions given by (II), *and*

for $1 \leq i \leq n-3$, and $i+1 < j \leq n-1$,

if $q_{\rho(i+1)\rho(j)} \leq q_{\rho(i)\rho(j+1)}$, then $q_{\rho(i+1)\rho(j)} = q_{\rho(i)\rho(j)}$ implies $q_{\rho(i+1)\rho(j+1)} = q_{\rho(i)\rho(j+1)}$, and $q_{\rho(i+1)\rho(j)} = q_{\rho(i+1)\rho(j+1)}$ implies $q_{\rho(i)\rho(j)} = q_{\rho(i)\rho(j+1)}$;

if $q_{\rho(i+1)\rho(j)} \geq q_{\rho(i)\rho(j+1)}$, then $q_{\rho(i)\rho(j+1)} = q_{\rho(i+1)\rho(j+1)}$ implies $q_{\rho(i)\rho(j)} = q_{\rho(i+1)\rho(j)}$, and $q_{\rho(i)\rho(j)} = q_{\rho(i)\rho(j+1)}$ implies $q_{\rho(i+1)\rho(j)} = q_{\rho(i+1)\rho(j+1)}$,

and for $2 \leq i \leq n-2$,

if $q_{\rho(i+1)\rho(n)} \leq q_{\rho(i)\rho(1)}$, then $q_{\rho(i+1)\rho(n)} = q_{\rho(i)\rho(n)}$ implies $q_{\rho(i+1)\rho(1)} = q_{\rho(i)\rho(1)}$, and $q_{\rho(i+1)\rho(n)} = q_{\rho(i+1)\rho(1)}$ implies $q_{\rho(i)\rho(n)} = q_{\rho(i)\rho(1)}$;

if $q_{\rho(i+1)\rho(n)} \geq q_{\rho(i)\rho(1)}$, then $q_{\rho(i)\rho(1)} = q_{\rho(i+1)\rho(1)}$ implies $q_{\rho(i)\rho(n)} = q_{\rho(i+1)\rho(n)}$, and $q_{\rho(i)\rho(n)} = q_{\rho(i)\rho(1)}$ implies $q_{\rho(i+1)\rho(n)} = q_{\rho(i+1)\rho(1)}$.

Again, the imposition of the stronger CSAR conditions avoids the type of graphical anomaly present in Figure 9.1(b) but now in the context of a CAR matrix — when two fitted values that are adjacent within a row are equal, the fitted values in the same two adjacent columns must also be equal for a row that is either its immediate predecessor (if $q_{\rho(i+1)\rho(j)} \leq q_{\rho(i)\rho(j+1)}$), or successor (if $q_{\rho(i+1)\rho(j)} \geq q_{\rho(i)\rho(j+1)}$); a similar condition is imposed when two fitted values that are adjacent within a column are equal. As noted, any SAR matrix is CSAR but not conversely.

The computational strategy we suggest for identifying a best-fitting CAR or CSAR approximation matrix is based on an initial circular unidimensional scaling obtained through the optimization strategy developed by Hubert, Arabie, and Meulman (1997) that is reviewed in Part I, Chapter 3. Specifically, by a combination of combinatorial search for good matrix reorderings, and heuristic iterative projection to locate the points of inflection when minimum distance calculations change directionality around a closed circular structure, approximation matrices to **P** are found through a least-squares loss criterion, and they have the parameterized form

$$\mathbf{Q}_\rho = \{\min(\mid x_{\rho(j)} - x_{\rho(i)} \mid,\ x_0 - \mid x_{\rho(j)} - x_{\rho(i)} \mid)\ + c\},$$

where c is an estimated additive constant, $x_{\rho(1)} \leq x_{\rho(2)} \leq \cdots \leq x_{\rho(n)} \leq x_0$, and the last coordinate, x_0, is the circumference of the circular structure. Based on the inequality constraints implied by such a collection of coordinates, a CAR approximation matrix can be fitted to **P** directly; then, beginning with this latter CAR approximation, the identification and imposition of CSAR constraints proceeds through the heuristic use of iterative projection, directly analogous to the way SAR constraints in the linear ordering context were identified and fitted, beginning with a best approximation matrix satisfying just the AR restrictions.

10.1 Fitting a Given CAR Matrix in the L_2-Norm

The MATLAB function m-file, `cirarobfit.m`, fits a circular anti-Robinson (CAR) matrix using iterative projection to a symmetric proximity matrix in the L_2-norm. Usage syntax is

```
[fit, vaf] = cirarobfit(prox,inperm,targ)
```

where `PROX` is the input proximity matrix ($n \times n$ with a zero main diagonal and a dissimilarity interpretation); `INPERM` is a given permutation of the first n integers (around a circle); `TARG` is a given $n \times n$ matrix having the circular anti-Robinson form that guides the direction in which distances are taken around the circle. The matrix `FIT` is the least-squares optimal approximation (with variance-accounted-for of `VAF`) to `PROX` having an circular anti-Robinson form for the row and column object ordering given by `INPERM`.

A recording of a MATLAB session follows that uses the `number.dat` data file; an equally-spaced circular anti-Robinson matrix `targcir` obtained from the utility m-file `ransymat.m` first introduced in Part I; and the identity permutation for the objects around the circular structure. The fitted CAR matrix identified in this way has a `vaf` of 64.37%.

```
 load number.dat
 [prox10 targlin targcir] = ransymat(10);
 [fit vaf] = cirarobfit(number,1:10,targcir)


fit =
  Columns 1 through 7

         0    0.4210    0.5840    0.6510    0.6835    0.8040    0.7730
    0.4210         0    0.2840    0.3460    0.6170    0.6170    0.7730
    0.5840    0.2840         0    0.2753    0.2753    0.5460    0.5460
    0.6510    0.3460    0.2753         0    0.2753    0.3844    0.3844
    0.6835    0.6170    0.2753    0.2753         0    0.3844    0.3844
    0.8040    0.6170    0.5460    0.3844    0.3844         0    0.3844
    0.7730    0.7730    0.5460    0.3844    0.3844    0.3844         0
    0.7695    0.7695    0.7960    0.5920    0.5530    0.4000    0.3857
    0.6597    0.6597    0.6597    0.8040    0.5530    0.5530    0.3857
    0.6510    0.6510    0.6510    0.6510    0.6835    0.5920    0.3857

  Columns 8 through 10

    0.7695    0.6597    0.6510
    0.7695    0.6597    0.6510
    0.7960    0.6597    0.6510
    0.5920    0.8040    0.6510
    0.5530    0.5530    0.6835
    0.4000    0.5530    0.5920
    0.3857    0.3857    0.3857
         0    0.3857    0.3857
    0.3857         0    0.3857
    0.3857    0.3857         0


vaf =

    0.6437
```

10.2 Finding a CAR Matrix in the L_2-Norm

The m-file, `cirarobfnd.m`, is our suggested strategy for identifying a best- fitting CAR matrix for a symmetric proximity matrix in the L_2-norm based on a permutation that is initially identified through the use of iterative quadratic assignment. Based on an equally-spaced circular target matrix, `order.m` is first invoked to obtain a good (circular) permutation, which is then used to construct a new circular target matrix with `cirfit.m`. (We will mention here but not illustrate with an example, an alternative to the use of `cirarobfnd.m` called `cirarobfnd_ac.m`; the latter m-file has the same syntax as `cirarobfnd.m` but uses `cirfitac.m` rather than `cirfit.m` internally to obtain the new circular target matrices.) The final output is generated from `cirarobfit.m` once it is determined that no better permutation can be identified using the newer circular target matrix. The usage syntax for `cirarobfnd.m` is as follows:

```
[fit, vaf, outperm] = cirarobfnd(prox, inperm, kblock)
```

where `PROX` is the input proximity matrix ($n \times n$ with a zero main diagonal and a dissimilarity interpretation); `INPERM` is a given starting permutation (assumed to be around the circle) of the first n integers; `FIT` is the least-squares optimal matrix (with variance-accounted-for of `VAF`) to `PROX` having a circular anti-Robinson form for the row and column object ordering given by the ending permutation `OUTPERM`. Again, `KBLOCK` defines the block size in the use of the iterative quadratic assignment routine.

An example of the use of `cirarobfnd.m` is given below that seems to lead to a circular ordering best interpreted according to the structural properties of the digits. This is only one of several local optima identifiable by repeated use of the routine from other random starting permutations. In general, the different local optima observed differ in the way the odd digits, $\{3, 5, 7, 9\}$, and the even digits, $\{2, 4, 6, 8\}$, are ordered within these sets when moving clockwise around a circular structure. Explicitly, all local optima had a general structure of $\rightarrow 0 \rightarrow 1 \rightarrow \{3, 5, 7, 9\} \rightarrow \{2, 4, 6, 8\} \rightarrow$, but with some variation in order within the odd and even digits. For example, the CAR matrix given below uses the odd digits as $\rightarrow 3 \rightarrow 5 \rightarrow 9 \rightarrow 7 \rightarrow$ and the even digits as $\rightarrow 6 \rightarrow 8 \rightarrow 4 \rightarrow 2. \rightarrow$.

```
[fit, vaf, outperm] = cirarobfnd(number, randperm(10), 3)

fit =

  Columns 1 through 7

         0    0.3460    0.5315    0.5315    0.6069    0.8040    0.4460
    0.3460         0    0.4210    0.4340    0.6069    0.7895    0.7895
    0.5315    0.4210         0    0.4340    0.6069    0.7895    0.7895
    0.5315    0.4340    0.4340         0    0.0590    0.3670    0.4210
    0.6069    0.6069    0.6069    0.0590         0    0.2460    0.3880
    0.8040    0.7895    0.7895    0.3670    0.2460         0    0.3500
    0.4460    0.7895    0.7895    0.4210    0.3880    0.3500         0
    0.4460    0.6300    0.9090    0.7697    0.6069    0.3960    0.3907
    0.4160    0.6250    0.8500    0.7698    0.6069    0.3960    0.3907
    0.4160    0.5880    0.7698    0.7698    0.6069    0.6069    0.4160

  Columns 8 through 10

    0.4460    0.4160    0.4160
    0.6300    0.6250    0.5880
    0.9090    0.8500    0.7698
    0.7697    0.7698    0.7698
    0.6069    0.6069    0.6069
    0.3960    0.3960    0.6069
    0.3907    0.3907    0.4160
         0    0.3907    0.4160
    0.3907         0    0.4160
    0.4160    0.4160         0


vaf =

    0.8128


outperm =

     4     2     1     3     5     9     7     8    10     6
```

10.3 Fitting and Finding a Strongly Circular-Anti-Robinson (SCAR) Matrix in the L_2-Norm

The two m-functions, (`cirsarobfit.m`) and (`cirsarobfnd.m`), are direct analogues of `cirarobfit.m` and `cirarobfnd.m`, respectively, but are concerned with fitting and finding *strongly* circular-anti-Robinson forms. The syntax for `cirsarobfit.m`, which fits a strongly anti-Robinson matrix using iterative projection to a symmetric proximity matrix in the L_2-norm, is

```
[fit, vaf] = cirsarobfit(prox, inperm, targ)
```

where, again, `PROX` is the input proximity matrix ($n \times n$ with a zero main diagonal and a dissimilarity interpretation); `INPERM` is a given permutation of the first n integers; `TARG` is a given $n \times n$ matrix having the circular anti-Robinson form that guides the direction in which distances are taken around the circle. `FIT` is the least-squares optimal matrix (with variance-accounted-for of `VAF`) to `PROX` having a strongly circular-anti-Robinson form for the row and column object ordering given by `INPERM`.

An example follows using the same identity permutation as was done in fitting a CAR form with `cirarobfit.m`; as might be expected from using the more restrictive SCAR form, the variance-accounted-for drops to .4501 from .6437.

```
[fit, vaf] = cirsarobfit(number,1:10,targcir)


fit =
  Columns 1 through 7

         0    0.4210    0.5840    0.6505    0.6505    0.6505    0.6505
    0.4210         0    0.2840    0.6505    0.6505    0.6505    0.6505
    0.5840    0.2840         0    0.2753    0.2753    0.4306    0.4306
    0.6505    0.6505    0.2753         0    0.2753    0.4306    0.4306
    0.6505    0.6505    0.2753    0.2753         0    0.4306    0.4306
    0.6505    0.6505    0.4306    0.4306    0.4306         0    0.4306
    0.6505    0.6505    0.4306    0.4306    0.4306    0.4306         0
    0.6505    0.6505    0.6505    0.6505    0.6505    0.6505    0.3857
    0.6505    0.6505    0.6505    0.6505    0.6505    0.6505    0.3857
    0.6505    0.6505    0.6505    0.6505    0.6505    0.6505    0.3857

  Columns 8 through 10

    0.6505    0.6505    0.6505
    0.6505    0.6505    0.6505
    0.6505    0.6505    0.6505
    0.6505    0.6505    0.6505
    0.6505    0.6505    0.6505
    0.6505    0.6505    0.6505
    0.3857    0.3857    0.3857
         0    0.3857    0.3857
    0.3857         0    0.3857
    0.3857    0.3857         0


vaf =

    0.4501
```

The m-function `cirsarobfnd.m`, which finds and fits a SCAR matrix using iterative projection to a symmetric proximity matrix in the L_2-norm based on a permutation identified through the use of iterative quadratic assignment, has the expected syntax

```
[fit, vaf, outperm] = cirsarobfnd(prox, inperm, kblock)
```

where, again, `PROX` is the input proximity matrix ($n \times n$ with a zero main diagonal and a dissimilarity interpretation); `INPERM` is a given starting permutation of the first n integers; `FIT` is the least-squares optimal matrix (with variance-accounted-for of `VAF`) to `PROX` having a circular strongly anti-Robinson form for the row and column object ordering given by the ending permutation `OUTPERM`. As usual, `KBLOCK` defines the block size in the use the iterative quadratic assignment routine. (Analogous to the last section, an alternative to `cirsarobfnd.m` is available, called `cirsarobfnd_ac.m`that uses `cirfitac.m` to obtain the circular target matrices.)

In the MATLAB recording below, and starting from a random permutation, a circular strongly anti-Robinson form was found with a variance-accounted-for of .7296 (again, this represents an expected drop from the value of .8119 for the CAR form — this is also listed below)).

```
[fit, vaf, outperm] = cirsarobfnd(number,randperm(10), 2)

target =

  Columns 1 through 6

         0    0.4160    0.4160    0.4160    0.6262    0.6262
    0.4160         0    0.3907    0.3907    0.3960    0.6263
    0.4160    0.3907         0    0.3907    0.3960    0.6263
    0.4160    0.3907    0.3907         0    0.3500    0.3880
    0.6262    0.3960    0.3960    0.3500         0    0.2460
    0.6262    0.6263    0.6263    0.3880    0.2460         0
    0.7858    0.7858    0.7858    0.4210    0.3670    0.0590
    0.7858    0.7858    0.9090    0.7895    0.7895    0.5810
    0.5880    0.6250    0.6300    0.7895    0.7895    0.5810
    0.4160    0.4160    0.4460    0.4460    0.8040    0.5810

  Columns 7 through 10

    0.7858    0.7858    0.5880    0.4160
    0.7858    0.7858    0.6250    0.4160
    0.7858    0.9090    0.6300    0.4460
    0.4210    0.7895    0.7895    0.4460
    0.3670    0.7895    0.7895    0.8040
    0.0590    0.5810    0.5810    0.5810
         0    0.4340    0.4340    0.5315
    0.4340         0    0.4210    0.5315
    0.4340    0.4210         0    0.3460
    0.5315    0.5315    0.3460         0


vaf =

    0.8119
```

```
outperm =

     6    10     8     7     9     5     3     1     2     4


fit =

  Columns 1 through 6

         0    0.4246    0.4246    0.4246    0.7304    0.7304
    0.4246         0    0.3907    0.3907    0.3960    0.7304
    0.4246    0.3907         0    0.3907    0.3960    0.7304
    0.4246    0.3907    0.3907         0    0.3500    0.3880
    0.7304    0.3960    0.3960    0.3500         0    0.2460
    0.7304    0.7304    0.7304    0.3880    0.2460         0
    0.7304    0.7304    0.7304    0.4210    0.3670    0.0590
    0.7304    0.7304    0.7304    0.7304    0.7304    0.5810
    0.7304    0.7304    0.7304    0.7304    0.7304    0.5810
    0.4246    0.4246    0.4246    0.4246    0.7304    0.5810

  Columns 7 through 10

    0.7304    0.7304    0.7304    0.4246
    0.7304    0.7304    0.7304    0.4246
    0.7304    0.7304    0.7304    0.4246
    0.4210    0.7304    0.7304    0.4246
    0.3670    0.7304    0.7304    0.7304
    0.0590    0.5810    0.5810    0.5810
         0    0.4340    0.4340    0.5315
    0.4340         0    0.4210    0.5315
    0.4340    0.4210         0    0.3460
    0.5315    0.5315    0.3460         0


vaf =

    0.7296


outperm =

     6    10     8     7     9     5     3     1     2     4
```

Table 10.1: The fifteen (nonredundant) subsets listed according to increasing diameter values are contiguous in the circular object ordering used to display the CSAR entries in Table 10.2.

subset	*diameter*	*subset*	*diameter*
{4,2}	1.63	{6,8,4,2}	3.41
{8,4}	2.55	{0,1}	3.41
{1,3}	3.04	{3,5,9,7,6}	3.43
{6,8}	3.06	{2,0,1}	3.47
{8,4,2}	3.14	{2,0,1,3}	3.95
{6,8,4}	3.25	{4,2,0,1,3}	4.20
{9,7,6}	3.26	{0,1,3,5,9,7,6,8,4,2}	4.93
{9,7,6,8}	3.29		

10.4 Representing SCAR Structures (Graphically)

As in the case of an AR or SAR matrix, the interpretation of the structure that may be represented by a CAR or CSAR matrix could proceed by first identifying those subsets and their diameters that emerge by increasing a threshold variable from the smallest fitted value. And in the case of a more restrictive CSAR matrix, this collection of subsets and their diameters can then be displayed by a graph where minimum length paths reconstruct the fitted values. To illustrate this graphical possibility on the transformed `number.dat` to mean 4.0 and variance 1.0 given in Hubert, Arabie, and Meulman (1998) — and used earlier to show the graphical representation of an SAR matrix — the fifteen (nonredundant) subsets identified from the CSAR matrix present in Table 10.2 are listed in Table 10.1 according to increasing diameter. Here, the structural properties of the digits are apparent (e.g., various subsets of the odd or even digits, or those that are multiples or powers of 2 or of 3), but some magnitude adjacencies can also be noted (e.g., $\{6, 7, 8, 9\}$, or subsets of $\{0, 1, 2, 3\}$). The graph adhering to the CSAR restrictions is given in Figure 10.1 and again minimum path lengths (that proceed up from a terminal node to an internal node and then back down to the other terminal node) can be used to reconstruct the fitted values in $\mathbf{Q}$.

In addition to searching for a best-fitting CSAR matrix directly, we might comment that the type of indirect approach mentioned in the introduction for the case of SAR approximations could also be considered, although we will not go into any of the details here. For example, based on a best-fitting CAR matrix, the additional constraints of a circular unidimensional scale could be identified and then imposed (in fact, this is our starting place in first obtaining the CAR approximation); or those of an ultrametric (which would lead to an SAR matrix that is trivially CSAR as well); or possibly, a collection of additive tree restrictions could be identified. In all cases, CSAR approximations would be automatically obtained.

Table 10.2: A circular strongly-anti-Robinson order-constrained least-squares approximations to the digit proximity data of Shepard *et al.* (1975).

digit	0	1	3	5	9	7	6	8	4	2
0	x	3.41	3.95	4.93	4.93	4.93	4.93	4.93	4.20	3.47
1	3.41	x	3.04	4.93	4.93	4.93	4.93	4.93	4.20	3.47
3	3.95	3.04	x	3.43	3.43	3.43	3.43	4.93	4.20	3.95
5	4.93	4.93	3.43	x	3.43	3.43	3.43	4.93	4.93	4.93
9	4.93	4.93	3.43	3.43	x	3.26	3.26	3.29	4.93	4.93
7	4.93	4.93	3.43	3.43	3.26	x	3.26	3.29	4.93	4.93
6	4.93	4.93	3.43	3.43	3.26	3.26	x	3.06	3.25	3.41
8	4.93	4.93	4.93	4.93	3.29	3.29	3.06	x	2.55	3.14
4	4.20	4.20	4.20	4.93	4.93	4.93	3.25	2.55	x	1.63
2	3.47	3.47	3.95	4.93	4.93	4.93	3.41	3.14	1.63	x

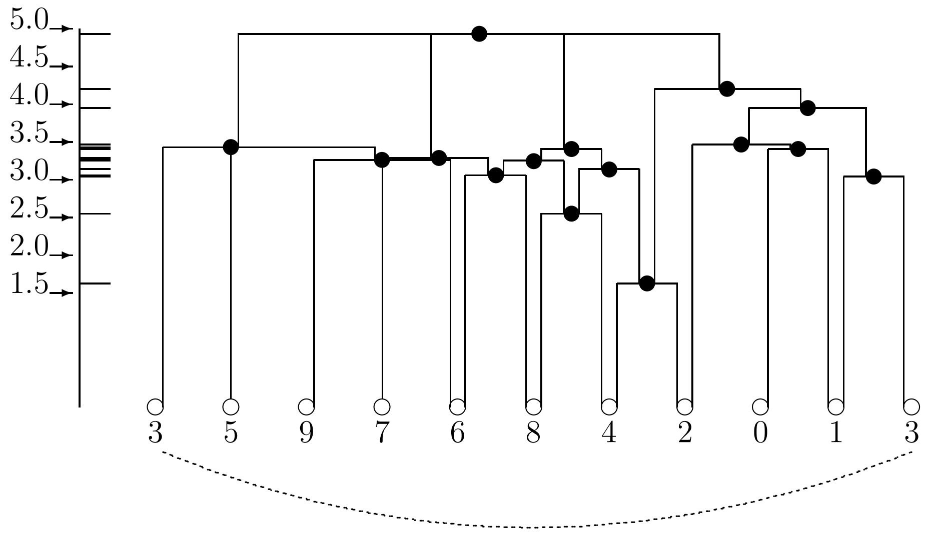


Figure 10.1: A graphical representation for the fitted values given by the circular strongly-anti-Robinson matrix in the lower-triangular portion of Table 10.2 (Vaf = 72.96%). Note that digit 3 is placed both in the first and the last positions in the ordering of the objects with the implication that the sequence continues in a circular manner. This circularity is indicated by the curved dashed line in the figure.

10.5 Representation Through Multiple (Strongly) CAR Matrices

Just as we discussed in Section 9.6 on representing proximity matrices through multiple (strongly) AR matrices, representations of a proximity matrix by a single (strongly) circular-anti-Robinson structure extends easily to the additive use of multiple matrices. The m-function, `bicirarobfnd.m`, fits the sum of two circular-anti-Robinson matrices using iterative projection to a symmetric proximity matrix in the L_2-norm based on permutations identified through the use of iterative quadratic assignment. The syntax usage is

```
[find,vaf,targone,targtwo,outpermone,outpermtwo] = ...
bicirarobfnd(prox,inperm,kblock)
```

where, as before, `PROX` is the input proximity matrix ($n \times n$ with a zero main diagonal and a dissimilarity interpretation); `INPERM` is a given starting permutation of the first n integers; `FIND` is the least-squares optimal matrix (with variance-accounted-for of `VAF`) to `PROX` and is the sum of the two circular-anti-Robinson matrices `TARGONE` and `TARGTWO` based on the two row and column object orderings given by the ending permutations `OUTPERMONE` and `OUTPERMTWO`. As before, `KBLOCK` defines the block size in the use of iterative quadratic assignment routine.

```
[find,vaf,targone,targtwo,outpermone,outpermtwo] = ...
bicirarobfnd(number,randperm(10),1)

find =

  Columns 1 through 7

         0    0.3837    0.5644    0.7286    0.6958    0.8352    0.8003
    0.3837         0    0.3410    0.3461    0.6645    0.5880    0.7576
    0.5644    0.3410         0    0.3342    0.0588    0.6710    0.4211
    0.7286    0.3461    0.3342         0    0.4330    0.4257    0.3000
    0.6958    0.6645    0.0588    0.4330         0    0.4090    0.3881
    0.8352    0.5880    0.6710    0.4257    0.4090         0    0.4257
    0.8003    0.7576    0.4211    0.3000    0.3881    0.4257         0
    0.9091    0.6489    0.8293    0.5920    0.6900    0.4000    0.4537
    0.8003    0.8003    0.3669    0.8040    0.2459    0.6900    0.3501
    0.8501    0.6063    0.7434    0.3114    0.6645    0.5175    0.2476

  Columns 8 through 10

    0.9091    0.8003    0.8501
    0.6489    0.8003    0.6063
    0.8293    0.3669    0.7434
    0.5920    0.8040    0.3114
    0.6900    0.2459    0.6645
    0.4000    0.6900    0.5175
    0.4537    0.3501    0.2476
         0    0.4046    0.4537
    0.4046         0    0.4046
    0.4537    0.4046         0


vaf =

    0.9836


targone =

  Columns 1 through 7

         0    0.4520    0.4520    0.4520    0.4520    0.6303    0.6303
    0.4520         0    0.4520    0.4520    0.4520    0.6303    0.6303
    0.4520    0.4520         0    0.3882    0.3882    0.3882    0.6303
    0.4520    0.4520    0.3882         0    0.3882    0.3882    0.6303
    0.4520    0.4520    0.3882    0.3882         0    0.3337    0.4143
    0.6303    0.6303    0.3882    0.3882    0.3337         0    0.1862
    0.6303    0.6303    0.6303    0.6303    0.4143    0.1862         0
    0.5314    0.7696    0.7696    0.7696    0.4473    0.3072    0.2560
    0.5314    0.7696    0.8337    0.8927    0.7839    0.7839    0.6303
    0.3723    0.5224    0.6325    0.6325    0.7839    0.7839    0.6303

  Columns 8 through 10

    0.5314    0.5314    0.3723
    0.7696    0.7696    0.5224
    0.7696    0.8337    0.6325
    0.7696    0.8927    0.6325
    0.4473    0.7839    0.7839
    0.3072    0.7839    0.7839
    0.2560    0.6303    0.6303
         0    0.3673    0.3673
    0.3673         0    0.3673
    0.3673    0.3673         0
```

```
targtwo =

  Columns 1 through 7

         0   -0.0520    0.0597    0.0656    0.0656    0.0656   -0.0262
   -0.0520         0    0.0164    0.0164    0.0164    0.0656    0.0656
    0.0597    0.0164         0    0.0164    0.0164    0.0164    0.0164
    0.0656    0.0164    0.0164         0    0.0164    0.0164    0.0164
    0.0656    0.0164    0.0164    0.0164         0   -0.0262   -0.0262
    0.0656    0.0656    0.0164    0.0164   -0.0262         0   -0.1406
   -0.0262    0.0656    0.0164    0.0164   -0.0262   -0.1406         0
   -0.0262    0.1400    0.1737    0.1972   -0.0262   -0.1406   -0.1520
   -0.0986    0.0597    0.0597    0.1972   -0.0262   -0.0262   -0.0262
   -0.2213    0.0597    0.0597    0.0656    0.0342    0.0342   -0.0262

  Columns 8 through 10

   -0.0262   -0.0986   -0.2213
    0.1400    0.0597    0.0597
    0.1737    0.0597    0.0597
    0.1972    0.1972    0.0656
   -0.0262   -0.0262    0.0342
   -0.1406   -0.0262    0.0342
   -0.1520   -0.0262   -0.0262
         0   -0.1972   -0.1972
   -0.1972         0   -0.1972
   -0.1972   -0.1972         0


outpermone =

     4     6    10     8     7     9     5     3     1     2


outpermtwo =

     6     8     9     1     2    10     7     4     3     5
```

For finding multiple SCAR forms, `bicirsarobfnd.m` has usage syntax

```
[find,vaf,targone,targtwo,outpermone,outpermtwo] = ...
```

```
bicirsarobfnd(prox,inperm,kblock)
```

with all the various terms the same as for `bicirarobfnd.m` but now for strongly CAR (SCAR) structures. The example below finds essentially the same representation as above (involving digit magnitude and structure) with a slight drop in the variance-accounted-for of 99.06%.

```
>> [find,vaf,targone,targtwo,outpermone,outpermtwo] = ...
bicirsarobfnd(number,randperm(10),1)

find =

  Columns 1 through 7

         0    0.4210    0.4841    0.6812    0.6812    0.8082    0.8082
    0.4210         0    0.3839    0.3459    0.5831    0.7100    0.6466
    0.4841    0.3839         0    0.3540    0.0589    0.6330    0.4211
    0.6812    0.3459    0.3540         0    0.5061    0.3740    0.3000
    0.6812    0.5831    0.0589    0.5061         0    0.4090    0.3879
    0.8082    0.7100    0.6330    0.3740    0.4090         0    0.4510
    0.8082    0.6466    0.4211    0.3000    0.3879    0.4510         0
    0.9090    0.8082    0.8082    0.5492    0.7179    0.4589    0.4445
    0.8082    0.7797    0.3672    0.7797    0.2460    0.6710    0.3502
    0.8082    0.6250    0.7080    0.3876    0.7100    0.4510    0.2829

  Columns 8 through 10

    0.9090    0.8082    0.8082
    0.8082    0.7797    0.6250
    0.8082    0.3672    0.7080
    0.5492    0.7797    0.3876
    0.7179    0.2460    0.7100
    0.4589    0.6710    0.4510
    0.4445    0.3502    0.2829
         0    0.3652    0.4445
    0.3652         0    0.4271
    0.4445    0.4271         0


vaf =

    0.9145
```

```
targone =

  Columns 1 through 7

         0    0.1456    0.5927    0.5927    0.5927    0.7197    0.7197
    0.1456         0    0.3956    0.3956    0.5927    0.7197    0.7197
    0.5927    0.3956         0    0.3325    0.5927    0.7197    0.7197
    0.5927    0.3956    0.3325         0    0.4190    0.7197    0.7197
    0.5927    0.5927    0.5927    0.4190         0    0.4607    0.4607
    0.7197    0.7197    0.7197    0.7197    0.4607         0    0.4607
    0.7197    0.7197    0.7197    0.7197    0.4607    0.4607         0
    0.7197    0.7197    0.7197    0.7197    0.4607    0.4607    0.3560
    0.3976    0.4328    0.7197    0.7197    0.4607    0.4607    0.3560
    0.2947    0.3072    0.7197    0.7197    0.7197    0.7197    0.3670

  Columns 8 through 10

    0.7197    0.3976    0.2947
    0.7197    0.4328    0.3072
    0.7197    0.7197    0.7197
    0.7197    0.7197    0.7197
    0.4607    0.4607    0.7197
    0.4607    0.4607    0.7197
    0.3560    0.3560    0.3670
         0    0.3560    0.3670
    0.3560         0    0.2902
    0.3670    0.2902         0


targtwo =

  Columns 1 through 7

         0   -0.0731   -0.0731   -0.0117   -0.0097   -0.0097    0.0600
   -0.0731         0   -0.1607   -0.0117   -0.0097   -0.0097    0.0600
   -0.0731   -0.1607         0   -0.2387   -0.0867   -0.0867    0.0600
   -0.0117   -0.0117   -0.2387         0   -0.0867   -0.0867    0.0600
   -0.0097   -0.0097   -0.0867   -0.0867         0   -0.3107   -0.0487
   -0.0097   -0.0097   -0.0867   -0.0867   -0.3107         0   -0.0487
    0.0600    0.0600    0.0600    0.0600   -0.0487   -0.0487         0
    0.0885    0.0885    0.0885    0.0885   -0.0018   -0.0018   -0.0018
    0.0885    0.0885    0.0885    0.0885    0.0885    0.0885    0.0885
   -0.0947   -0.0731   -0.0731   -0.0117   -0.0097   -0.0097    0.0600

  Columns 8 through 10

    0.0885    0.0885   -0.0947
    0.0885    0.0885   -0.0731
    0.0885    0.0885   -0.0731
    0.0885    0.0885   -0.0117
   -0.0018    0.0885   -0.0097
   -0.0018    0.0885   -0.0097
   -0.0018    0.0885    0.0600
         0    0.1893    0.0885
    0.1893         0    0.0885
    0.0885    0.0885         0


outpermone =

     5     3     1     2     4     6    10     8     7     9


outpermtwo =

    10     7     4     3     5     6     9     8     1     2
```

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