

Notes on Canonical Correlation

Suppose we have a collection of random variables in a $(q + p) \times 1$ vector \mathbf{X} that we partition in the following form (and supposing without loss of generality that $p \leq q$):

$$\mathbf{X} = \begin{pmatrix} X_1 \\ \vdots \\ X_p \\ \text{---} \\ X_{p+1} \\ \vdots \\ X_{p+q} \end{pmatrix} = \begin{pmatrix} \mathbf{X}_1 \\ \text{---} \\ \mathbf{X}_2 \end{pmatrix} \sim \text{MVN}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) ,$$

where

$$\boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{pmatrix} ; \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{pmatrix} ,$$

and remembering that $\boldsymbol{\Sigma}_{21} = \boldsymbol{\Sigma}'_{12}$, and

$$\text{Cor}(\mathbf{a}'\mathbf{X}_1, \mathbf{b}'\mathbf{X}_2) = \mathbf{a}'\boldsymbol{\Sigma}_{12}\mathbf{b} / \sqrt{\mathbf{a}'\boldsymbol{\Sigma}_{11}\mathbf{a}}\sqrt{\mathbf{b}'\boldsymbol{\Sigma}_{22}\mathbf{b}} .$$

Suppose

$$\boldsymbol{\Sigma}_{11}^{-1}\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}'_{12}\mathbf{a} = \lambda\mathbf{a} ,$$

with roots $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p \geq 0$, and corresponding eigenvectors $\mathbf{a}_1, \dots, \mathbf{a}_p$. Also, let

$$\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}'_{12}\boldsymbol{\Sigma}_{11}^{-1}\boldsymbol{\Sigma}_{12}\mathbf{b} = \lambda\mathbf{b} ,$$

with roots $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p \geq 0$ and $\lambda_{p+1} = \lambda_q = 0$; the corresponding eigenvectors are $\mathbf{b}_1, \dots, \mathbf{b}_p$.

Looking at the two linear combinations, $\mathbf{a}'_i \mathbf{X}_1$ (called the i^{th} canonical variate in the first set), and $\mathbf{b}'_i \mathbf{X}_2$ (called the i^{th} canonical variate in the second set), the squared correlation between them is λ_i ; the i^{th} canonical correlation is $\sqrt{\lambda_i}$. The maximum correlation between any two linear combinations is $\sqrt{\lambda_1}$, and is obtained for \mathbf{a}_1 and \mathbf{b}_1 . For \mathbf{a}_i and \mathbf{b}_i , these are uncorrelated with every canonical variate up to that point, and maximize the correlation subject to that restriction.

Points to make:

a) The matrices $\Sigma_{11}^{-1} \Sigma_{12} \Sigma_{22}^{-1} \Sigma'_{12}$ and $\Sigma_{22}^{-1} \Sigma'_{12} \Sigma_{11}^{-1} \Sigma_{12}$ are not symmetric and so the standard eigenvector/eigenvalue decompositions are not straightforward. However, the two matrices

$$\Sigma_{11}^{-1/2} \Sigma_{12} \Sigma_{22}^{-1} \Sigma'_{12} \Sigma_{11}^{-1/2}$$

and

$$\Sigma_{22}^{-1/2} \Sigma'_{12} \Sigma_{11}^{-1} \Sigma_{12} \Sigma_{22}^{-1/2}$$

are symmetric. Also,

$$\Sigma_{11}^{-1/2} \Sigma_{12} \Sigma_{22}^{-1} \Sigma'_{12} \Sigma_{11}^{-1/2} \mathbf{e}_i = \lambda_i \mathbf{e}_i ,$$

and

$$\Sigma_{22}^{-1/2} \Sigma'_{12} \Sigma_{11}^{-1} \Sigma_{12} \Sigma_{22}^{-1/2} \mathbf{f}_i = \lambda_i \mathbf{f}_i ,$$

where the roots, i.e., the λ_i s, are the same as before. We can then obtain $\mathbf{a}_i = \Sigma_{11}^{-1/2} \mathbf{e}_i$, and $\mathbf{b}_i = \Sigma_{22}^{-1/2} \mathbf{f}_i$. Both $\Sigma_{11}^{-1/2}$ and $\Sigma_{22}^{-1/2}$ are constructed from the spectral decompositions of $\Sigma_{11} = \mathbf{PDP}'$ and $\Sigma_{22} = \mathbf{QFQ}'$ as $\Sigma_{11}^{-1/2} = \mathbf{PD}^{-1/2} \mathbf{P}'$ and $\Sigma_{22}^{-1/2} = \mathbf{QF}^{-1/2} \mathbf{Q}'$. Note

the normalizations of $\text{Var}(\mathbf{a}'_i \mathbf{X}_1) = \mathbf{a}'_i \boldsymbol{\Sigma}_{11} \mathbf{a}_i = \mathbf{e}'_i \boldsymbol{\Sigma}_{11}^{-1/2} \boldsymbol{\Sigma}_{11} \boldsymbol{\Sigma}_{11}^{-1/2} \mathbf{e}_i = 1$ and $\text{Var}(\mathbf{b}'_i \mathbf{X}_2) = 1$.

b) There are three different normalizations that are commonly used for \mathbf{a}_i and \mathbf{b}_i :

(i) leave as unit length so $\mathbf{a}'_i \mathbf{a}_i = \mathbf{b}'_i \mathbf{b}_i = 1$;

(ii) make the largest value 1.0 in both \mathbf{a}_i and \mathbf{b}_i ;

(iii) do as we did above and make $\mathbf{a}'_i \boldsymbol{\Sigma}_{11} \mathbf{a}_i = 1 = \mathbf{b}'_i \boldsymbol{\Sigma}_{22} \mathbf{b}_i$.

(c) Special cases: When $p = 1$ and $q = 1$, λ_1 is the (simple) squared correlation between two variables; when $p = 1$ and $q > 1$, λ_1 is a squared multiple correlation. In considering $\mathbf{a}'_i \mathbf{X}_1$ versus \mathbf{X}_2 , λ_i is the squared multiple correlation of $\mathbf{a}'_i \mathbf{X}_1$ with \mathbf{X}_2 ; \mathbf{b}_i gives the regression weights.

(d) When moving to the sample, all items have direct analogues. The one restriction on sample size is $n \geq p + q + 1$.

(e) Suppose the variables \mathbf{X}_1 and \mathbf{X}_2 are transformed by nonsingular matrices, $\mathbf{A}_{p \times p}$ and $\mathbf{B}_{q \times q}$, as follows:

$$\mathbf{Y}_1 = \mathbf{A}_{p \times p} \mathbf{X}_1 + \mathbf{c}_{p \times 1}$$

$$\mathbf{Y}_2 = \mathbf{B}_{q \times q} \mathbf{X}_2 + \mathbf{d}_{q \times 1}$$

The same canonical variates and correlations using \mathbf{Y}_1 and \mathbf{Y}_2 would be generated as from \mathbf{X}_1 and \mathbf{X}_2 ; the weights in \mathbf{a}_i and \mathbf{b}_i would be on the transformed variables, obviously. In particular, we could work with standardized variables without loss of any generality, and just use the correlation matrix.

(f) To evaluate $H_0 : \boldsymbol{\Sigma}_{12} = \mathbf{0}$, a likelihood ratio test is available:

$$-(n - 1 - (1/2)(p + q + 1)) \ln \prod_{i=1}^p (1 - \lambda_i) \sim \chi_{pq}^2 .$$

Also, sometimes a sequential process is used to test the remaining roots until nonsignificance is reached:

$$-(n - 1 - (1/2)(p + q + 1)) \ln \prod_{i=k+1}^p (1 - \lambda_i) \sim \chi_{(p-k)(q-k)}^2 .$$

This latter sequential procedure is a little problematic because there is no real control over the overall significance level with this strategy.

Generally, there is some tortuous difficulty in interpreting the canonical weights substantively. I might suggest using a constrained least-squares approach (iteratively moving from one set to a second), where the weights are forced to be nonnegative.