

# Statistics 135

## Chapter 10

### Canonical Correlations

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# Purpose of Canonical Correlations

Principal components (PCA) is used to investigate one set of variables. The original variables are replaced by a set of variables called principal components which are created to account for maximal variation among the original variables. Canonical correlations is a generalization of PCA with the goal to identify and quantify the associations between two sets of variables.

- 1 Two vectors  $\mathbf{X}_{p \times 1}^{(1)}$  and  $\mathbf{X}_{q \times 1}^{(2)}$  with  $p \leq q$ .
- 2 Focus is on the correlation between a linear combination of one set of variables  $\mathbf{X}^{(1)}$  and the linear combination of another set of variables  $\mathbf{X}^{(2)}$ .
- 3 Determine the pair of linear combinations with the largest correlation
- 4 Next, determine a pair of linear combinations having the largest correlation among pairs uncorrelated with the initial pair and so on.

We assume the following model:

$$\begin{aligned} E(\mathbf{X}^{(1)}) &= \mu^{(1)} & Cov(\mathbf{X}^{(1)}) &= \Sigma^{11} \\ E(\mathbf{X}^{(2)}) &= \mu^{(2)} & Cov(\mathbf{X}^{(2)}) &= \Sigma^{22} \end{aligned}$$

$$Cov(\mathbf{X}^{(1)}, \mathbf{X}^{(2)}) = \Sigma_{12} = \Sigma'_{21}$$

Let  $U, V$  be linear combinations of  $\mathbf{X}^{(1)}$  and  $\mathbf{X}^{(2)}$  where

$$U = \mathbf{a}'\mathbf{X}^{(1)} \quad \text{and} \quad V = \mathbf{b}'\mathbf{X}^{(2)}$$

then

$$\begin{aligned} Var(U) &= \mathbf{a}'\Sigma_{11}\mathbf{a} & \text{and} & & Var(V) &= \mathbf{b}'\Sigma_{22}\mathbf{b} \\ Cov(U, V) &= \mathbf{a}'\Sigma_{12}\mathbf{b} \end{aligned}$$

We are interested in finding  $\mathbf{a}$  and  $\mathbf{b}$  which maximize

$$Corr(U, V) = \frac{\mathbf{a}'\Sigma_{12}\mathbf{b}}{\sqrt{\mathbf{a}'\Sigma_{11}\mathbf{a}}\sqrt{\mathbf{b}'\Sigma_{22}\mathbf{b}}} \tag{1}$$

- 1 The first pair of canonical variables  $U_1, V_1$  maximizes (1) subject to  $Var(U_1) = Var(V_1) = 1$
- 2 The second pair of canonical variables  $U_2, V_2$  maximizes (1) subject to

$$Var(U_2) = Var(V_2) = 1$$

$$Cov(U_1, U_2) = Cov(V_1, V_2) = Cov(U_1, V_2) = Cov(U_2, V_1) = 0$$

- 3 The  $k^{th}$  canonical pair is given by

$$U_k = \mathbf{e}_k' \Sigma_{11}^{-1/2} \mathbf{X}^{(1)} \quad \text{and} \quad V_k = \mathbf{f}_k' \Sigma_{22}^{-1/2} \mathbf{X}^{(2)}$$

$$Corr(U_k, V_k) = \rho^*$$

- 4  $\rho_1^* > \rho_2^* > \dots > \rho_p^*$  are the eigenvalues of  $\Sigma_{11}^{-1/2} \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} \Sigma_{11}^{-1/2}$  and  $\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_p$  are the associated eigenvectors;
- 5  $\rho_1^* > \rho_2^* > \dots > \rho_p^*$  are also the p largest eigenvalues (out of  $q > p$ ) of  $\Sigma_{22}^{-1/2} \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12} \Sigma_{22}^{-1/2}$  with eigenvectors  $\mathbf{f}_1, \mathbf{f}_2, \dots, \mathbf{f}_q$

# Calculation and Interpretation

- 1 Split the  $(p + q) \times (p + q)$  covariance matrix of  $(\mathbf{X}'_1, \mathbf{X}'_2)'$  into  $\Sigma_{11}$ ,  $\Sigma_{12}$  and  $\Sigma_{22}$
- 2 Calculate  $\Sigma_{11}^{-1/2} \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21} \Sigma_{11}^{-1/2}$
- 3 Obtain the eigenvalues  $\rho_j^*$  for  $j = 1, \dots, p$  and the associated eigenvectors  $\mathbf{e}_j$ .
- 4 For the eigenvalues in (3) obtain the eigenvectors  $\mathbf{f}_1, \dots, \mathbf{f}_q$  (only the first  $p$  are needed) of  $\Sigma_{22}^{-1/2} \Sigma_{21} \Sigma_{11}^{-1} \Sigma_{12} \Sigma_{22}^{-1/2}$ , this matrix as its  $p$  largest has eigenvalues  $\rho_1^*, \dots, \rho_p^*$ , the other eigenvalues are  $\rho_{p+1}^*, \dots, \rho_q^*$ .
- 5 Form the linear combinations  $U_k = \mathbf{e}_k \Sigma_{11}^{-1/2} \mathbf{X}^{(1)}$  and  $V_k = \mathbf{f}_k \Sigma_{22}^{-1/2} \mathbf{X}^{(2)}$  for  $k = 1, \dots, p$ .
- 6 Continue until the canonical correlation  $\rho_k^*$  is very small.

- 7 Let  $\mathbf{U} = \mathbf{A}\mathbf{X}^{(1)}$  and  $\mathbf{V} = \mathbf{B}\mathbf{X}^{(2)}$  where  $\mathbf{A} = \mathbf{E}'\mathbf{\Sigma}_{11}^{-1/2}$  and  $\mathbf{B} = \mathbf{F}'\mathbf{\Sigma}_{22}^{-1/2}$ .  
Then

$$Cov(\mathbf{U}) = \mathbf{A}\mathbf{\Sigma}_{11}\mathbf{A}' = \mathbf{I} \quad \text{and} \quad Cov(\mathbf{V}) = \mathbf{B}\mathbf{\Sigma}_{11}\mathbf{B}' = \mathbf{I}$$

- 8 Since  $\mathbf{\Sigma}_{11} = \mathbf{P}_1\mathbf{\Lambda}\mathbf{P}_1'$  we can write

$$\mathbf{U} = \mathbf{A}\mathbf{X}^{(1)} = \mathbf{E}'\mathbf{P}_1\mathbf{\Lambda}^{-1/2}\mathbf{P}_1'\mathbf{X}^{(1)}$$

and we have a similar expression for  $\mathbf{V}$ . Therefore,  $\mathbf{U}$  can be interpreted as

- a a transformation of  $\mathbf{X}^{(1)}$  to uncorrelated principal components followed by
- b a rigid rotation  $\mathbf{P}_1$  determined by  $\mathbf{\Sigma}_{11}$  followed by
- c another rotation  $\mathbf{E}'$  determined from the full covariance matrix  $\mathbf{\Sigma}$  of  $\mathbf{X}^{(1)}, \mathbf{X}^{(2)}$ .

# Estimation

When we have a sample  $(\mathbf{x}_1^{(1)}, \mathbf{x}_1^{(2)}), \dots, (\mathbf{x}_1^{(1)}, \mathbf{x}_1^{(2)})$ , then we calculate the sample mean vector  $\bar{\mathbf{x}}^{(1)}, \bar{\mathbf{x}}^{(2)}$  and the sample covariance matrix

$$\mathbf{S} = \begin{pmatrix} \mathbf{S}_{11} & \mathbf{S}_{12} \\ \mathbf{S}_{21} & \mathbf{S}_{22} \end{pmatrix}$$

The calculations outlined in items (1) through (6) in the calculation section are then carried out for the sample covariance or correlation matrix.

A test for a diagonal covariance matrix  $H_0 : \Sigma_{12} = \mathbf{0}$  is given by

$$-2\ln\Lambda = n \ln\left(\frac{|\mathbf{S}_{11}| |\mathbf{S}_{22}|}{|\mathbf{S}|}\right) = -n \ln \prod_{i=1}^p (1 - \hat{\rho}_i^{*2})$$

which has a  $\chi_{pq}^2$  distribution. An improved version is

$$-\left(n - 1 - \frac{1}{2}(p + q + 1)\right) \ln \prod_{i=1}^p (1 - \hat{\rho}_i^{*2})$$