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Canonical Correlation Analysis

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Synonyms

[Canonical analysis](#); [Canonical variate analysis](#); [External factor analysis](#).

Glossary

Canonical correlation Correlation between two canonical variates of the same pair. This is the criterion optimized by CCA.

Canonical loadings Correlation between the original variables and the canonical variates. Sometimes used as a synonym for canonical vectors (because these quantities differ only by their normalization).

Canonical variates The latent variables (one per data table) computed in CCA (also called canonical variables, canonical variable scores, or canonical factor scores). The canonical variates have maximal correlation.

Canonical vectors The set of coefficients of the linear combinations used to compute the canonical variates, also called canonical *weights*. Canonical vectors are also sometimes called canonical loadings.

Latent variable A linear combination of the variables of one data table. In general, a latent variable is computed to satisfy some predefined criterion.

Definition

Canonical correlation analysis (CCA) is a statistical method whose goal is to extract the information common to two data tables that measure quantitative variables on a same set of observations. To do so, CCA creates pairs of linear combinations of the variables (one per table) that have maximal correlation.

Introduction

Originally defined by Hotelling in 1935 (Hotteling 1935; Hotteling 1936, see also Bartlett 1948), canonical correlation analysis (CCA) is a statistical method whose goal is to extract the information common to two data tables that measure quantitative variables on a same set of observations. To do so, CCA computes two sets of linear combinations – called *latent variables* – (one for each data table) that have maximum correlation. To visualize this common information extracted by the analysis, a convenient way is (1) to plot the latent variables of one set against the other set (this creates plots akin to plots of factor scores in principal component analysis); (2) to plot the coefficients of the linear combinations (this creates plots akin to plotting the loadings in principal component analysis); and (3) to plot the correlations between the original variables and the latent variables (this creates correlation circle” plots like in principal component analysis).

CCA generalizes many standard statistical techniques (e.g., multiple regression, analysis of variance, discriminant analysis) and can also be declined in several related methods that address slightly different types of problems (e.g., different normalization conditions, different types of data).

Key Points

CCA extracts the information common to two data tables measuring quantitative variables on the same set of observations. For each data table, CCA computes a set of linear combinations of the variables of this table called *latent variables* or *canonical variates* with the constraints that a latent variable from one table has maximal correlation with one latent variable of the other table and no correlation with the remaining latent variables of the other table. The results of the analysis are interpreted using different types of graphical displays that plot the latent variables and the coefficients of the linear combinations used to create the latent variables.

Historical Background

After principal component analysis (PCA), CCA is one of the oldest multivariate techniques that was first defined in 1935 by Hotelling. In addition of being the first method created for the statistical analysis of two data tables, CCA is also of theoretical interest because a very large number of linear multivariate analytic tools are particular cases of CCA. Like most multivariate statistical techniques, CCA has been really feasible only with the advent of modern computers. Recent developments involve generalization of CCA to the case of more than two-tables and cross-validation approaches to select important variables and the stability and reliability of the solution obtained on a given sample.

Canonical Correlation Analysis

Notations

Matrices are denoted in upper case bold letters, vectors are denoted in lower case bold, and their elements are denoted in lower case italic. Matrices, vectors, and elements from the same matrix all use the same letter (e.g., \mathbf{A} , \mathbf{a} , a). The transpose operation is denoted by the superscript^T, the inverse operation is denoted by ⁻¹. The identity matrix is denoted \mathbf{I} , vectors or matrices of ones are denoted $\mathbf{1}$, and matrices or vectors of zeros are denoted $\mathbf{0}$. When provided with a square matrix, the diag operator gives a vector with the diagonal elements of this matrix. When provided with a vector, the diag operator gives a diagonal matrix with the elements of the vector as the diagonal elements of this matrix. When provided with a square matrix, the trace operator gives the sum of the diagonal elements of this matrix.

The data tables to be analyzed by CCA of, respectively, size $N \times I$ and $N \times J$, are denoted \mathbf{X} and \mathbf{Y} and collect two sets of, respectively, I and J quantitative measurements obtained on the same N observations. Except if mentioned otherwise, matrices \mathbf{X} and \mathbf{Y} are column centered and normalized, and so:

$$\mathbf{1}^\top \mathbf{X} = \mathbf{0}, \mathbf{1}^\top \mathbf{Y} = \mathbf{0}, \quad (1)$$

(with $\mathbf{1}$ being a conformable vector of 1 s and $\mathbf{0}$ a conformable vector of 0 s), and

$$\text{diag}\{\mathbf{X}^\top, \mathbf{X}\} = \mathbf{1}, \text{diag}\{\mathbf{Y}^\top, \mathbf{Y}\} = \mathbf{1}. \quad (2)$$

Note that because \mathbf{X} and \mathbf{Y} are centered and normalized matrices, their inner products are correlation matrices that are denoted:

$$\begin{aligned} \mathbf{R}_X &= \mathbf{X}^\top \mathbf{X}, & \mathbf{R}_Y &= \mathbf{Y}^\top \mathbf{Y} & \text{and} \\ \mathbf{R} &= \tilde{\mathbf{X}}^\top \mathbf{Y}. \end{aligned} \quad (3)$$

Optimization Problem

In CCA, the problem is to find two latent variables, denoted \mathbf{f} and \mathbf{g} obtained as linear combinations of the columns of, respectively, \mathbf{X} and \mathbf{Y} . The coefficients of these linear combinations are stored, respectively, in the $I \times 1$ vector \mathbf{p} and the $J \times 1$ vector \mathbf{q} ; and, so, we are looking for

$$\mathbf{f} = \mathbf{X}\mathbf{p} \text{ and } \mathbf{g} = \mathbf{Y}\mathbf{q}. \quad (4)$$

In CCA, we want the latent variables to have maximum *correlation* and so we are looking for \mathbf{p} and \mathbf{q} satisfying:

$$\begin{aligned} \delta &= \arg \max_{\mathbf{p}, \mathbf{q}} \{\text{cor}(\mathbf{f}, \mathbf{g})\} \\ &= \arg \max_{\mathbf{p}, \mathbf{q}} \left\{ \frac{\mathbf{f}^\top \mathbf{g}}{\sqrt{(\mathbf{f}^\top \mathbf{f}) (\mathbf{g}^\top \mathbf{g})}} \right\}. \end{aligned} \quad (5)$$

The correlation between latent variables – maximized by CCA – is called the *canonical correlation* (Gittins 2012; Hotteling 1936; Horst, 1961; Mardia et al. 1980).

An easy way to solve the maximization problem of CCA is to constraint the latent variables to have unitary norm (because, in this case, the term $\mathbf{f}^\top \mathbf{g}$ gives the correlation between \mathbf{f} and \mathbf{g}). Specifically, we require that:

$$\begin{aligned} \mathbf{f}^\top \mathbf{f} &= \mathbf{p}^\top \mathbf{X}^\top \mathbf{X} \mathbf{p} = \mathbf{p}^\top \mathbf{R}_X \mathbf{p} = 1 = \mathbf{g}^\top \mathbf{g} \\ &= \mathbf{q}^\top \mathbf{Y}^\top \mathbf{Y} \mathbf{q} = \mathbf{q}^\top \mathbf{R}_Y \mathbf{q}. \end{aligned} \quad (6)$$

With these notations, the maximization problem from Eq. 5 becomes:

$$\begin{aligned} \arg \max_{\mathbf{p}, \mathbf{q}} \{ \mathbf{f}^\top \mathbf{g} = \mathbf{p}^\top \mathbf{R} \mathbf{q} \} & \text{ under the constraints that} \\ \mathbf{p}^\top \mathbf{R}_X \mathbf{p} = 1 &= \mathbf{q}^\top \mathbf{R}_Y \mathbf{q}. \end{aligned} \quad (7)$$

Equivalent Optimum Criteria

The maximization problem expressed in Eq. 5 can also be expressed as the following equivalent minimization problem:

$$\arg \max_{\mathbf{p}, \mathbf{q}} \{ \| \mathbf{X}\mathbf{p} - \mathbf{Y}\mathbf{q} \|_2^2 \} =$$

$$\arg \max_{\mathbf{p}, \mathbf{q}} \{ \text{trace}\{(\mathbf{X}\mathbf{p} - \mathbf{Y}\mathbf{q})^\top (\mathbf{X}\mathbf{p} - \mathbf{Y}\mathbf{q})\} \}$$

$$\text{under the constraints that } \mathbf{p}^\top \mathbf{R}_X \mathbf{p} = 1 = \mathbf{q}^\top \mathbf{R}_Y \mathbf{q}. \quad (8)$$

Lagrangian Approach

A standard way to solve the type of maximization described in Eq. 7 is to use a Lagrangian approach. To do so we need: first to define a Lagrangian that incorporates the constraints; next, to take the derivative of the Lagrangian respective to the unknown quantities (here: \mathbf{p} and \mathbf{q}); and, finally, to set the derivative to zero in order to obtain the normal equations. Solving the normal equations will then give the values of the parameters that solve the optimization problem (i.e., for CCA: maximum correlation).

Here the Lagrangian (denoted \mathcal{L}) that includes the constraints with the two Lagrange multipliers α and β is

$$\begin{aligned} \mathcal{L} &= \mathbf{p}^\top \mathbf{R} \mathbf{q} - \alpha (\mathbf{p}^\top \mathbf{R}_X \mathbf{p} - 1) \\ &\quad - \beta (\mathbf{q}^\top \mathbf{R}_Y \mathbf{q} - 1). \end{aligned} \quad (9)$$

The derivatives of the Lagrangian for \mathbf{p} and \mathbf{q} are

$$\frac{\partial \mathcal{L}}{\partial \mathbf{p}} = \mathbf{R}\mathbf{q} - 2\alpha\mathbf{R}_X\mathbf{p} \quad (10)$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{q}} = \mathbf{R}^\top\mathbf{p} - 2\beta\mathbf{R}_Y\mathbf{q}. \quad (11)$$

The Normal Equations

Setting Eqs. 10 and 11 to zero gives the normal equations:

$$\mathbf{R}\mathbf{q} = 2\alpha\mathbf{R}_X\mathbf{p} \quad (12)$$

$$\mathbf{R}^\top\mathbf{p} = 2\beta\mathbf{R}_Y\mathbf{q}. \quad (13)$$

Solution of the Normal Equations

The first step to solve the normal equations is to show that $\alpha = \beta$. This is done by premultiplying Eq. 12 by \mathbf{p} and Eq. 13 by \mathbf{q} to obtain (using the constraints from Eq. 3):

$$\mathbf{p}^\top\mathbf{R}\mathbf{q} = 2\alpha\mathbf{p}^\top\mathbf{R}_X\mathbf{p} = 2\alpha \quad (14)$$

$$\mathbf{q}^\top\mathbf{R}^\top\mathbf{p} = 2\beta\mathbf{q}^\top\mathbf{R}_Y\mathbf{q} = 2\beta \quad (15)$$

Equating $\mathbf{p}^\top\mathbf{R}\mathbf{q}$ and $\mathbf{q}^\top\mathbf{R}^\top\mathbf{p}$ shows that $2\alpha = 2\beta$. For convenience, in what follows we set $\delta = 2\alpha = 2\beta$.

Postmultiplying Eq. 12 by \mathbf{R}_X^{-1} and Eq. 13 by \mathbf{R}_Y^{-1} gives

$$\mathbf{R}_X^{-1}\mathbf{R}\mathbf{q} = \delta\mathbf{p} \quad (16)$$

$$\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{p} = \delta\mathbf{q}. \quad (17)$$

Replacing \mathbf{q} (respectively \mathbf{p}) in Eq. 16 (respectively Eq. 17) by its expression from Eq. 17 (respectively Eq. 16) gives the following two eigen-equations (see Abdi 2007b) for a refresher about the eigen-decomposition):

$$\mathbf{R}_X^{-1}\mathbf{R}\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{p} = \delta^2\mathbf{p} \quad (18)$$

$$\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{R}_X^{-1}\mathbf{R}\mathbf{q} = \delta^2\mathbf{q}, \quad (19)$$

which shows that \mathbf{p} (respectively \mathbf{q}) is the eigenvector of the nonsymmetric matrix $\mathbf{R}_X^{-1}\mathbf{R}\mathbf{R}_Y^{-1}\mathbf{R}^\top$

(respectively, $\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{R}_X^{-1}\mathbf{R}$), associated with the first eigenvalue $\lambda_1 = \delta^2$, and that the maximum correlation (i.e., the *canonical* correlation) is equal to δ . Note that in order to make explicit the constraints expressed in Eq. 7, the vectors \mathbf{p} and \mathbf{q} are normalized (respectively) in the metric \mathbf{R}_X and \mathbf{R}_Y (i.e., $\mathbf{p}^\top\mathbf{R}_X\mathbf{p} = 1$ and $\mathbf{q}^\top\mathbf{R}_Y\mathbf{q} = 1$).

Additional Pairs of Latent Variables

After the first pair of latent variables has been found, additional pairs of latent variables can be extracted. The criterion from Eqs. 5 and 7 is still used for the subsequent pairs of latent variables, along with the requirement that the new latent variables are orthogonal to the previous ones. Specifically, if \mathbf{f}_ℓ and \mathbf{g}_ℓ denote the ℓ -th pair of latent variables, the orthogonality condition becomes:

$$\mathbf{f}_\ell^\top\mathbf{f}_{\ell'} = 0 \quad \text{and} \quad \mathbf{g}_\ell^\top\mathbf{g}_{\ell'} = 0 \quad \forall \ell \neq \ell'. \quad (20)$$

This orthogonality condition imposed on the latent variables is equivalent to imposing an \mathbf{R}_X - (respectively \mathbf{R}_Y -) orthogonality condition on the eigenvectors \mathbf{p} and \mathbf{q} , namely that:

$$\mathbf{p}_\ell^\top\mathbf{R}_X\mathbf{p}_{\ell'} = 0 \quad \text{and} \quad \mathbf{q}_\ell^\top\mathbf{R}_Y\mathbf{q}_{\ell'} = 0 \quad \forall \ell \neq \ell'. \quad (21)$$

For convenience, latent variables and eigenvectors can be stored in matrices \mathbf{F} , \mathbf{G} , \mathbf{P} , and \mathbf{Q} . With these notations, the normalization (from Eq. 7) and orthogonality (from Eq. 21) conditions are written as

$$\mathbf{F}^\top\mathbf{F} = \mathbf{I} \Leftrightarrow \mathbf{P}^\top\mathbf{R}_X\mathbf{P} = \mathbf{I} \quad (22)$$

$$\mathbf{G}^\top\mathbf{G} = \mathbf{I} \Leftrightarrow \mathbf{Q}^\top\mathbf{R}_Y\mathbf{Q} = \mathbf{I}. \quad (23)$$

The matrices of eigenvectors \mathbf{P} and \mathbf{Q} are respectively called \mathbf{R}_X - and \mathbf{R}_Y - orthogonal (the proof of this property is given in the next section, see Eq. 27).

The eigen-decompositions for \mathbf{P} and \mathbf{Q} can then be expressed in a matrix form as:

$$\mathbf{R}_X^{-1}\mathbf{R}\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{P}=\mathbf{P}\mathbf{\Lambda} \quad \text{and} \quad \mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{R}_X^{-1}\mathbf{R}\mathbf{Q}=\mathbf{Q}\mathbf{\Lambda}. \quad (24)$$

Solution from the Eigen-Decomposition of Symmetric Matrices

The matrices \mathbf{P} and \mathbf{Q} can also be obtained from the decomposition of two symmetric matrices. For example, matrix \mathbf{P} can be obtained from the following eigendecomposition

$$\mathbf{R}_X^{-\frac{1}{2}}\mathbf{R}\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{R}_X^{-\frac{1}{2}}=\tilde{\mathbf{P}}\mathbf{\Lambda}\tilde{\mathbf{P}}^\top \quad \text{with} \quad \tilde{\mathbf{P}}^\top\tilde{\mathbf{P}}=\mathbf{I}. \quad (25)$$

This can be shown by first defining $\tilde{\mathbf{P}}=\mathbf{R}_X^{-\frac{1}{2}}\mathbf{P}$ and replacing \mathbf{P} by $\mathbf{R}_X^{-\frac{1}{2}}\tilde{\mathbf{P}}$ in Eq. 24 and then simplifying:

$$\begin{aligned} \mathbf{R}_X^{-1}\mathbf{R}\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{P} &= \mathbf{P}\mathbf{\Lambda} \\ \mathbf{R}_X^{-\frac{1}{2}}\mathbf{R}\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{R}_X^{-\frac{1}{2}}\tilde{\mathbf{P}} &= \mathbf{R}_X^{-\frac{1}{2}}\mathbf{P}\mathbf{\Lambda} \quad (\text{because } \mathbf{P}=\mathbf{R}_X^{-\frac{1}{2}}\tilde{\mathbf{P}}) \\ \mathbf{R}_X^{\frac{1}{2}}\mathbf{R}_X^{-1}\mathbf{R}\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{R}_X^{-\frac{1}{2}}\tilde{\mathbf{P}} &= \mathbf{R}_X^{\frac{1}{2}}\mathbf{R}_X^{-\frac{1}{2}}\mathbf{P}\mathbf{\Lambda} \\ & \quad (\text{Multiply both sides by } \mathbf{R}_X^{\frac{1}{2}}) \\ \mathbf{R}_X^{-\frac{1}{2}}\mathbf{R}\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{R}_X^{-\frac{1}{2}}\tilde{\mathbf{P}} &= \tilde{\mathbf{P}}\mathbf{\Lambda}. \end{aligned} \quad (26)$$

This shows that $\tilde{\mathbf{P}}$ is the matrix of the eigenvectors of the symmetric matrix $\mathbf{R}_X^{-\frac{1}{2}}\mathbf{R}\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{R}_X^{-\frac{1}{2}}$, which also implies that $\tilde{\mathbf{P}}^\top\tilde{\mathbf{P}}=\mathbf{I}$. The eigenvectors of the asymmetric matrix $\mathbf{R}_X^{-1}\mathbf{R}\mathbf{R}_Y^{-1}\mathbf{R}^\top$ are then recovered as $\mathbf{P}=\mathbf{R}_X^{-\frac{1}{2}}\tilde{\mathbf{P}}$. A simple substitution shows that \mathbf{P} is \mathbf{R}_X -orthogonal:

$$\mathbf{P}^\top\mathbf{R}_X\mathbf{P}=\tilde{\mathbf{P}}^\top\mathbf{R}_X^{-\frac{1}{2}}\mathbf{R}_X\mathbf{R}_X^{-\frac{1}{2}}\tilde{\mathbf{P}}=\tilde{\mathbf{P}}^\top\tilde{\mathbf{P}}=\mathbf{I}. \quad (27)$$

A similar derivation shows that \mathbf{Q} can be obtained from the eigen-decomposition

$$\mathbf{R}_Y^{-\frac{1}{2}}\mathbf{R}^\top\mathbf{R}_X^{-1}\mathbf{R}\mathbf{R}_Y^{-\frac{1}{2}}=\tilde{\mathbf{Q}}\mathbf{\Lambda}\tilde{\mathbf{Q}}^\top \quad (28)$$

with $\tilde{\mathbf{Q}}^\top\tilde{\mathbf{Q}}=\mathbf{I}$, where $\mathbf{Q}=\mathbf{R}_Y^{-\frac{1}{2}}\tilde{\mathbf{Q}}$.

Solution from One Singular Value Decomposition

The eigenvector matrices \mathbf{P} and \mathbf{Q} can also be obtained from the singular value decomposition (SVD, see, e.g., Greenacre (1984); Abdi (2007a)) of the matrix

$$\begin{aligned} \mathbf{R}_X^{-\frac{1}{2}}\mathbf{R}\mathbf{R}_Y^{-\frac{1}{2}} &= \tilde{\mathbf{P}}\mathbf{\Delta}\tilde{\mathbf{Q}}^\top = \sum_{\ell} \delta_{\ell}\tilde{\mathbf{p}}_{\ell}\tilde{\mathbf{q}}_{\ell} \\ \text{with } \tilde{\mathbf{P}}^\top\tilde{\mathbf{P}} &= \tilde{\mathbf{Q}}^\top\tilde{\mathbf{Q}} = \mathbf{I}. \end{aligned} \quad (29)$$

where $\tilde{\mathbf{P}}$, $\tilde{\mathbf{Q}}$, and $\mathbf{\Delta}$ denote (respectively) the left, right singular vectors, and a diagonal matrix of the singular values of matrix $\mathbf{R}_X^{-\frac{1}{2}}\mathbf{R}\mathbf{R}_Y^{-\frac{1}{2}}$. The matrices \mathbf{P} and \mathbf{Q} (containing the vectors \mathbf{p} and \mathbf{q}) are then computed as

$$\begin{aligned} \tilde{\mathbf{P}} &= \mathbf{R}_X^{\frac{1}{2}}\mathbf{P} \quad \text{and} \quad \tilde{\mathbf{Q}} = \mathbf{R}_Y^{\frac{1}{2}}\mathbf{Q} \Leftrightarrow \\ \mathbf{P} &= \mathbf{R}_X^{-\frac{1}{2}}\tilde{\mathbf{P}} \quad \text{and} \quad \mathbf{Q} = \mathbf{R}_Y^{-\frac{1}{2}}\tilde{\mathbf{Q}}. \end{aligned} \quad (30)$$

From the Eigen-Decomposition to the Singular Value Decomposition

To show that \mathbf{p} can be found from the eigen-decompositions from Eqs. 18 and 19, we first replace \mathbf{p} by $\tilde{\mathbf{p}}$ in Eq. 18. This gives:

$$\mathbf{R}_X^{-1}\mathbf{R}\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{R}_X^{-\frac{1}{2}}\tilde{\mathbf{p}} = \delta^2\tilde{\mathbf{p}}, \quad (31)$$

then premultiplying both sides of Eq. 31 by $\mathbf{R}_X^{\frac{1}{2}}$ and simplifying gives

$$\begin{aligned} \mathbf{R}_X^{\frac{1}{2}}\mathbf{R}_X^{-1}\mathbf{R}\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{R}_X^{-\frac{1}{2}}\tilde{\mathbf{p}} &= \delta^2\mathbf{R}_X^{\frac{1}{2}}\tilde{\mathbf{p}} \\ \Leftrightarrow \mathbf{R}_X^{-\frac{1}{2}}\mathbf{R}\mathbf{R}_Y^{-1}\mathbf{R}^\top\mathbf{R}_X^{-\frac{1}{2}}\tilde{\mathbf{p}} &= \delta^2\tilde{\mathbf{p}}. \end{aligned} \quad (32)$$

A similar argument shows that

$$\mathbf{R}_Y^{-\frac{1}{2}}\mathbf{R}^\top\mathbf{R}_X^{-1}\mathbf{R}\mathbf{R}_Y^{-\frac{1}{2}}\tilde{\mathbf{q}} = \delta^2\tilde{\mathbf{q}}. \quad (33)$$

Combining Eqs. 32 and 33 shows that $\tilde{\mathbf{p}}$ and $\tilde{\mathbf{q}}$ are left and right singular vectors of the matrix $\mathbf{R}_X^{-\frac{1}{2}}\mathbf{R}\mathbf{R}_Y^{-\frac{1}{2}}$.

An Example: The Colors and Grapes of Wines

To illustrate CCA we use the data set presented in Table 1. These data describe thirty-six red, rosé, or white wines produced in three different countries (Chili, Canada, and USA) using several different varietal of grapes. These wines are described by two different sets of variables. The first set of variables (i.e., matrix \mathbf{X}) describes the objective properties of the wines: Price, Acidity, Alcohol content, Sugar, and Tannin (in what follows we capitalize these descriptors). The second set of variables (i.e., matrix \mathbf{Y}) describes the subjective properties of the wines as evaluated by a professional wine taster and consists in ratings on a nine-point rating scale of eight aspects of taste: fruity, floral, vegetal, spicy, woody, sweet, astringent, acidic, plus an overall evaluation of the hedonic aspect of the wine (i.e., how much the taster liked the wine).

The analysis of this example was performed using the statistical programming language R and is available to download from <https://github.com/vguillemot/2Tables>.

Figures 1, 2, and 3 show heatmaps of the correlation matrices \mathbf{R}_X , \mathbf{R}_Y , and \mathbf{R} . As shown in Fig. 3 (for matrix \mathbf{R}), the objective variables alcohol and tannin are positively correlated with the perceived qualities of astringent and woody; by contrast, the perceived hedonic aspect of wine is negatively correlated with alcohol, tannin (and price, so our taster liked inexpensive wines) and positively correlated with the sugar content of the wines. Unsurprisingly, the objective amount of Sugar is correlated with the perceived quality sweet.

The CCA of these data found five pairs of latent variables [in general CCA will find a maximum of $\min(I, J)$ pairs of latent variables]. The values of the canonical correlations are shown in Fig. 4. The first and second canonical correlations are very high (.98 and .85, see Table 2), and so we will only consider them here. As shown in Figs. 5 and 6, the latent variables extracted by the analysis are very sensitive to “the color” of the wines: The first pair of latent variables (Fig. 5) isolates the red wines, whereas the second pair of latent variables

(Fig. 6) roughly orders the wines according to their concentration of red pigment (i.e., white, rosé, and red; similar plots using grape varietal or origin of the wines did not show any interesting patterns and are therefore not shown).

To understand the contribution of the variables of \mathbf{X} and \mathbf{Y} to the latent variables, two types of plots are used: (1) a plot of the correlation between latent variables and original variables and (2) a plot of the loadings of the variables. Figure 7 (respectively Figure 8) shows the correlation between the original variables (both \mathbf{X} and \mathbf{Y}) and respectively \mathbf{F} (i.e., the latent variables from \mathbf{X}) and \mathbf{G} (i.e., the latent variables from \mathbf{Y}). Figs. 9 and 10 display the loadings for, respectively, \mathbf{X} and \mathbf{Y} (i.e., matrices \mathbf{P} and \mathbf{Q}) for the first two dimensions of the analysis. Together these figures indicate that the first dimension reflects the negative correlation between Alcohol (from \mathbf{X}) and the subjective hedonic evaluation of the wines (from \mathbf{Y}), whereas the second dimension combines (low) Alcohol, (high) Acidity, and (high) Sugar (from \mathbf{X}) to reflect their correlations with the subjective variables astringent and hedonic. Figs. 7 and 8 show very similar pictures (because the latent variables are very correlated) and this suggests that the first pair of latent variables opposes “bitterness” (i.e., astringent, alcohol, etc.) to sweetness, whereas the second pair of latent variables opposes bitterness (from astringent) to the “burning” effect of Alcohol.

Variations over CCA

By imposing slightly different orthogonality conditions than the ones described in Eqs. 14 and 15, different (but related) alternative methods can be defined to analyze two data tables.

Inter-Battery Analysis (IBA) Et Alia

The oldest alternative – originally proposed by Tucker in 1958 – called inter-battery analysis (IBA) (Tucker 1958), is also known under a variety of different names such as coinertia analysis (Dolédec and Chessel 1994), partial least square SVD (PLSVD) (Bookstein 1994), partial least square correlation (PLSC) (Krishnan et al. 2010;

Canonical Correlation Analysis, Table 1 An example for CCA. Thirty-six wines are described by two sets of variables: objective descriptors (Matrix X) and subjective descriptors (Matrix Y)

Wine	Origin	Color	Varietal	Matrix X: Objective							Matrix Y: Subjective						
				Price	Acidity	Alcohol	Sugar	Tannin	Fruity	Floral	Vegetal	Spicy	Woody	Sweet	Astringent	Acidic	Hedonic
CH01	Chili	Red	Merlot	11	5.33	13.80	2.75	559	6	2	1	4	5	3	5	4	2
CH02	Chili	Red	Cabernet	5	5.14	13.90	2.41	672	5	3	2	3	4	2	6	3	2
CH03	Chili	Red	Shiraz	7	5.16	14.30	2.20	455	7	1	2	6	5	3	4	2	2
CH04	Chili	red	Pinot	16	4.37	13.50	3.00	348	5	3	2	2	4	1	3	4	4
CH05	Chili	White	Chardonnay	14	4.34	13.30	2.61	46	5	4	1	3	4	2	1	4	6
CH06	Chili	White	Sauvignon	8	6.60	13.30	3.17	54	7	5	6	1	1	4	1	5	8
CH07	Chili	White	Riesling	9	7.70	12.30	2.15	42	6	7	2	2	2	3	1	6	9
CH08	Chili	White	Gewurz	11	6.70	12.50	2.51	51	5	8	2	1	1	4	1	4	9
CH09	Chili	Rose	Malbec	4	6.50	13.00	7.24	84	8	4	3	2	2	6	2	3	8
CH10	Chili	Rose	Cabernet	3	4.39	12.00	4.50	90	6	3	2	1	1	5	2	3	8
CH11	Chili	Rose	Pinot	6	4.89	12.00	6.37	76	7	2	1	1	1	4	1	4	9
CH12	Chili	Rose	Syrah	5	5.90	13.50	4.20	80	8	4	1	3	2	5	2	3	7
CA01	Canada	Red	Merlot	20	7.42	14.90	2.10	483	5	3	2	3	4	3	4	4	3
CA02	Canada	Red	Cabernet	15	7.35	14.50	1.90	698	6	3	2	2	5	2	5	4	2
CA03	Canada	Red	Shiraz	20	7.50	14.50	1.50	413	6	2	3	4	3	3	5	1	2
CA04	Canada	Red	Pinot	25	5.70	13.30	1.70	320	4	2	3	3	1	3	2	4	4
CA05	Canada	White	Chardonnay	20	6.00	13.50	3.00	35	4	3	2	1	3	2	2	3	5
CA06	Canada	White	Sauvignon	15	7.50	12.00	3.50	40	8	4	3	2	1	3	1	4	8
CA07	Canada	White	Riesling	15	7.00	11.90	3.40	48	7	5	1	1	3	3	1	7	8
CA08	Canada	White	Gewurz	18	6.30	13.90	2.80	39	6	5	2	2	2	3	2	5	6
CA09	Canada	Rose	Malbec	8	5.90	12.00	5.50	90	6	3	3	3	2	4	2	4	8
CA10	Canada	Rose	Cabernet	6	5.60	12.50	4.00	85	5	4	1	3	2	4	2	4	7
CA11	Canada	Rose	Pinot	9	6.20	13.00	6.00	75	5	3	2	1	2	3	2	3	7
CA12	Canada	Rose	Syrah	9	5.80	13.00	3.50	83	7	3	2	3	3	4	1	4	7
US01	USA	Red	Merlot	25	6.00	13.60	3.50	578	7	2	2	5	6	3	4	3	2
US02	USA	Red	Cabernet	15	6.50	14.60	3.50	710	8	3	1	4	5	3	5	3	2

(continued)

Canonical Correlation Analysis, Table 1 (continued)

	Matrix X: Objective										Matrix Y: Subjective									
	USA	Red	Shiraz	25	5.30	13.90	1.99	610	8	2	3	7	6	4	5	3	1	1		
US03	USA	Red	Shiraz	25	5.30	13.90	1.99	610	8	2	3	7	6	4	5	3	1	1		
US04	USA	Red	Pinot	28	6.10	14.00	0.00	340	6	3	2	2	5	2	4	4	2	2		
US05	USA	White	Chardonnay	15	7.20	13.30	1.10	41	6	4	2	3	6	3	2	4	5	5		
US06	USA	White	Sauvignon	8	7.20	13.50	1.00	50	6	5	5	1	2	4	2	4	7	7		
US07	USA	White	Riesling	10	8.60	12.00	1.65	47	5	5	3	2	2	4	2	5	8	8		
US08	USA	White	Gewurz	20	9.60	12.00	0.00	45	6	6	3	2	2	4	2	3	8	8		
US09	USA	Rose	Malbec	3	6.20	12.50	4.00	84	8	2	1	4	3	5	2	4	7	7		
US10	USA	Rose	Cabernet	4	5.71	12.50	4.30	93	8	3	3	3	2	6	2	3	8	8		
US11	USA	Rose	Pinot	8	5.40	13.00	3.10	79	6	1	1	2	3	4	1	3	6	6		
US12	USA	Rose	Syrah	6	6.50	13.50	3.00	89	9	3	2	5	4	3	2	3	5	5		

Abdi and Williams 2013), singular value decomposition of the covariance between two fields (Bretherton et al. 1992), maximum covariance analysis (von Storch and Zwiers 2002), or even, recently, “multivariate genotype-phenotype” (MGP) analysis (Mitteroecker et al. 2016). It is particularly popular in brain-imaging and related domains (McIntosh et al. 1996). In IBA (like in CCA) the latent variables are obtained as linear combinations of the variables of \mathbf{X} and \mathbf{Y} but instead of having maximum correlation

(as described in Eqs. 5 and 7) the latent variables are required to have maximum *covariance*. So we are looking for vectors \mathbf{p} and \mathbf{q} satisfying:

$$\begin{aligned} \delta &= \arg \max_{\mathbf{p}, \mathbf{q}} \{ \text{cov}(\mathbf{f}, \mathbf{g}) \} \\ &= \arg \max_{\mathbf{p}, \mathbf{q}} \{ \mathbf{f}^T \mathbf{g} = \mathbf{p}^T \mathbf{R} \mathbf{q} \} \end{aligned} \quad (34)$$

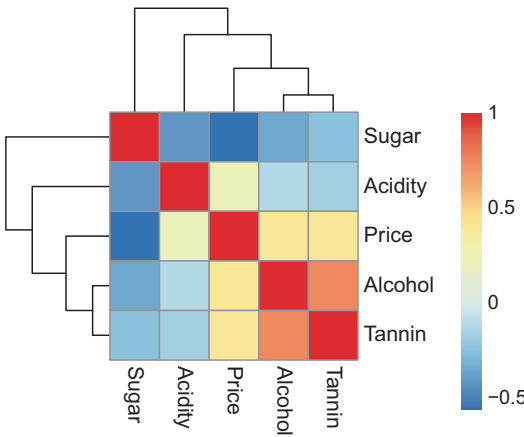
An easy way to solve this problem is to impose the constraints that \mathbf{p} and \mathbf{q} have unitary norm, namely that:

$$\mathbf{p}^T \mathbf{p} = 1 = \mathbf{q}^T \mathbf{q}. \quad (35)$$

A derivation similar to the one used for CCA shows that the coefficients \mathbf{P} and \mathbf{Q} and the optimal linear combination can be directly obtained from the singular decomposition of the correlation matrix \mathbf{R} as:

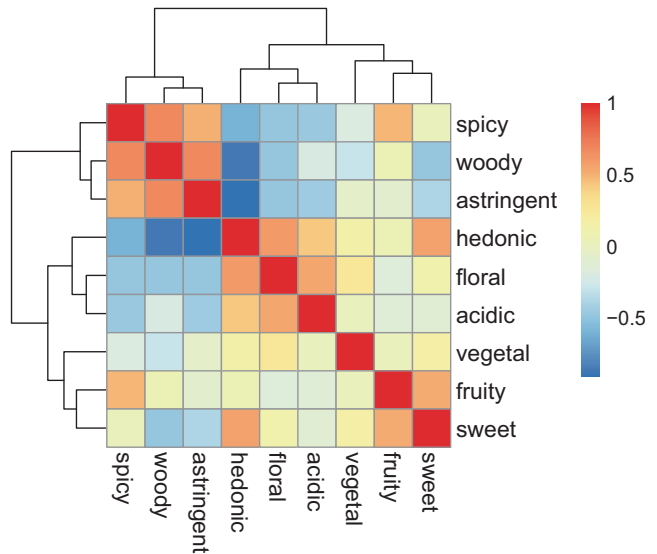
$$\begin{aligned} \mathbf{R} &= \mathbf{P} \mathbf{\Delta} \mathbf{Q}^T = \sum_{\ell} \delta_{\ell} \mathbf{p}_{\ell} \mathbf{q}_{\ell}^T \\ &\text{with } \mathbf{P}^T \mathbf{P} = \mathbf{Q}^T \mathbf{Q} = \mathbf{I}. \end{aligned} \quad (36)$$

where \mathbf{P} , \mathbf{Q} , and $\mathbf{\Delta}$ are (respectively) matrices containing the left, right singular vectors, and diagonal matrix of the singular values of \mathbf{R} .

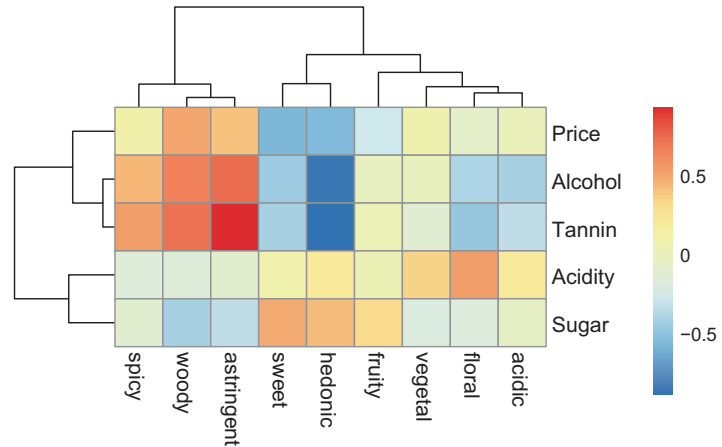


Canonical Correlation Analysis, Fig. 1 Heatmap of correlation matrix \mathbf{R}_X (i.e., between the variables of matrix \mathbf{X})

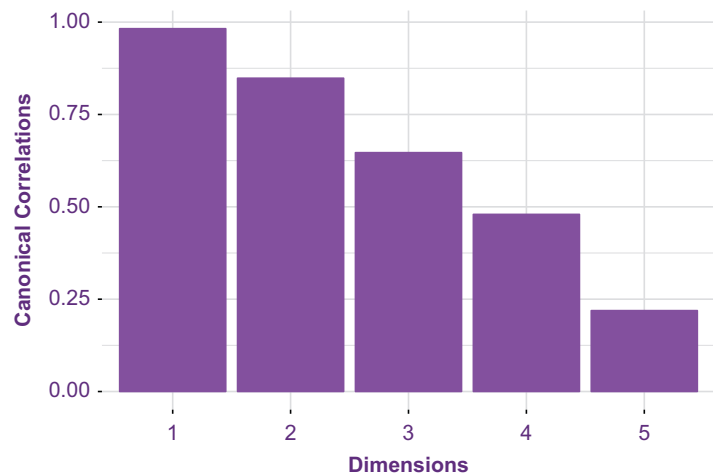
Canonical Correlation Analysis, Fig. 2 Heatmap of correlation matrix \mathbf{R}_Y (i.e., between the variables of matrix \mathbf{Y})



Canonical Correlation Analysis, Fig. 3 Heatmap of correlation matrix \mathbf{R} (i.e., between the variables of matrices \mathbf{X} and \mathbf{Y})



Canonical Correlation Analysis, Fig. 4 Barplot of the canonical correlations (i.e., correlations between pairs of latent variables for a given dimension)



Because IBA maximizes the *covariance* between latent variables (instead of the *correlation* for CCA), it does not require the inversion of matrices \mathbf{R}_X and \mathbf{R}_Y and therefore, IBA can be used with rank deficient or badly conditioned matrices and, in particular, when the number of observations is smaller than the number of variables (a configuration sometimes called $N \ll P$). This makes IBA a robust technique popular for domains using Big or “Wide” Data such as, for example, brain imaging (Krishnan et al. 2010; Grellmann et al. 2015) or genomics (Beaton et al. 2016).

Asymmetric Two-Table Analysis

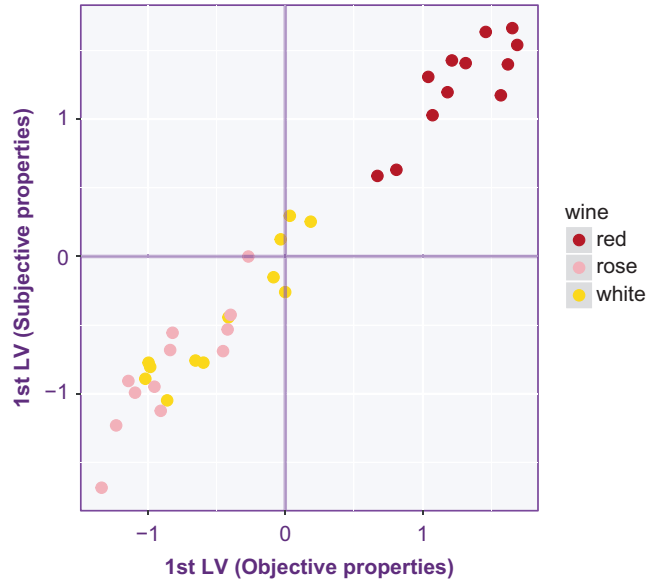
CCA and IBA are symmetric techniques because the results of the analysis will be unchanged (*mutatis mutandis*) if \mathbf{X} and \mathbf{Y} are permuted. Other related techniques differentiate the roles of \mathbf{X} and \mathbf{Y} and treat \mathbf{X} as a matrix of predictor variables and \mathbf{Y} as a matrix of dependent variables (i.e., to be “explained” or “predicted” by \mathbf{X}). Among these techniques, the two most well-known approaches are *redundancy analysis* and *partial least square regression* (see, also, Takane 2013, for alternative methods and review).

Canonical Correlation Analysis, Table 2 An example for CCA. Canonical correlations (δ_i), loadings for matrices **X** (objective descriptors, loading matrix **P**) and **Y** (subjective descriptors loading matrix **Q**) for the five dimensions extracted by CCA

Dimension	δ_i	Matrix P : Objective										Matrix Q : Subjective									
		Price	Acidity	Alcohol	Sugar	Tannin	Fruity	Floral	Vegetal	Spicy	Woody	Sweet	Astringent	Acidic	Hedonic						
1	.98	0.026	-0.088	0.489	-0.134	0.002	0.000	0.150	0.030	-0.068	-0.109	0.082	-0.095	0.059	-0.586						
2	.85	-0.062	0.306	-0.927	0.188	0.006	0.274	-0.247	-0.150	0.114	0.307	-0.285	1.688	0.085	1.179						
3	.65	-0.024	0.678	-0.243	-0.288	0.001	0.044	0.605	0.366	0.024	0.390	-0.133	0.465	-0.083	0.327						
4	.48	-0.057	0.574	1.382	0.428	-0.002	0.565	0.368	-0.076	-0.427	-0.505	0.584	-0.531	-0.423	-0.870						
5	.22	0.157	0.360	-0.131	0.627	-0.000	0.744	-0.205	0.087	-0.877	0.290	-0.568	0.296	0.065	0.185						

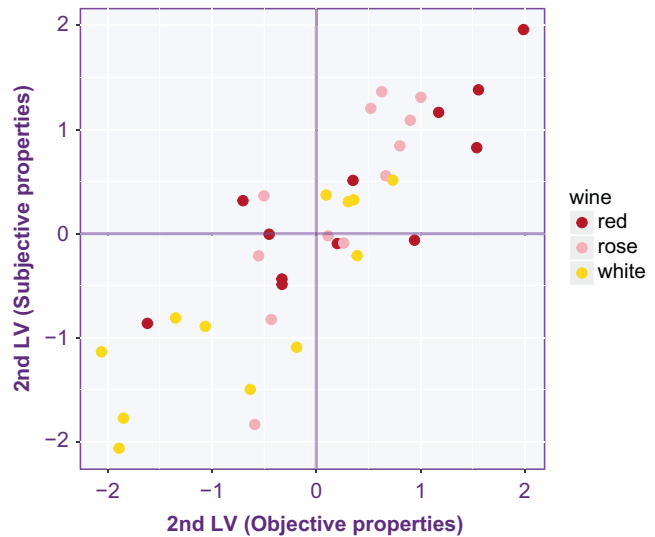
Canonical Correlation Analysis, Fig. 5 CCA.

Latent variables: First latent variable from \mathbf{X} (1st LV objective properties) vs. First latent variable from \mathbf{Y} (first LV subjective properties). One point represents one wine. Wines are colored according to their types (i.e., red, rosé, or white). Red wines are well separated from the other wines



Canonical Correlation Analysis, Fig. 6 CCA.

Latent variables: Second latent variable from \mathbf{X} (second LV objective properties) vs. Second latent variable from \mathbf{Y} (2nd LV subjective properties). One point represents one wine. Wines are colored according to their types (i.e., red, rosé, or white)



Redundancy Analysis

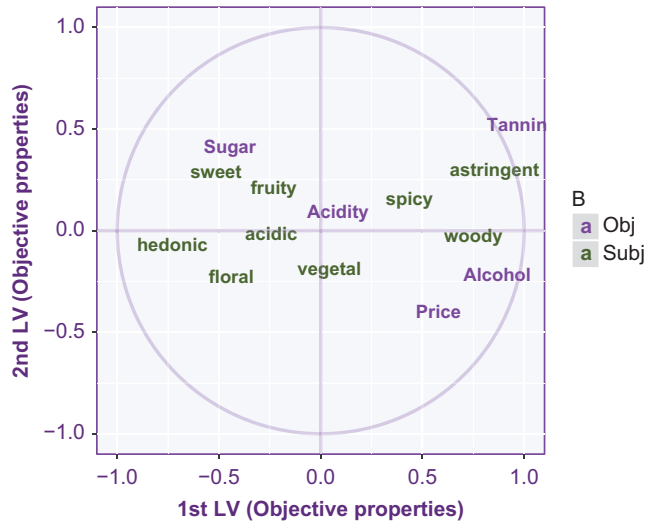
Redundancy analysis (RA, (Van Den Wollenberg 1977)) – originally developed under the name of *principal component analysis of instrumental variables* by Rao in 1964 (Rao 1964) and *simultaneous prediction method* (by Fortier 1966) – can be seen as a technique intermediate between CCA and IBA. In RA, the vectors stored in \mathbf{P} (i.e., the loadings from \mathbf{X} , the predictors) are required to be \mathbf{R}_X -normalized (just like in CCA) but the vectors stored in \mathbf{Q} (i.e., the loadings from \mathbf{Y} , the

predictors) are required to be unit normalized (just like in IBA). Specifically, RA is solving the following optimization problem:

$$\begin{aligned} \delta &= \operatorname{argmax}_{\mathbf{p}, \mathbf{q}} \{ \operatorname{cov}(\mathbf{f}, \mathbf{g}) \} \\ &= \operatorname{argmax}_{\mathbf{p}, \mathbf{q}} \{ \mathbf{f}^\top \mathbf{g} = \mathbf{p}^\top \mathbf{R} \mathbf{q} \} \\ &\text{with } \mathbf{p}^\top \mathbf{R}_X \mathbf{p} = 1 = \mathbf{q}^\top \mathbf{q}. \end{aligned} \quad (37)$$

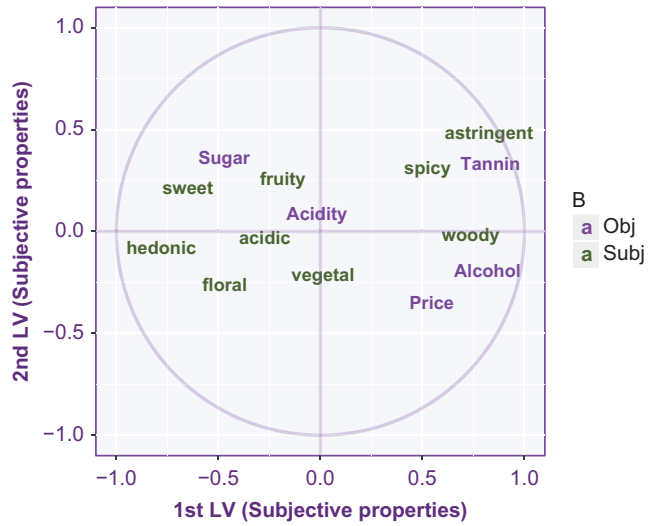
Canonical Correlation Analysis,

Fig. 7 Correlation circle with latent variables from matrix **X**



Canonical Correlation Analysis,

Fig. 8 Correlation circle with latent variables from matrix **Y**



RA can be interpreted as searching for the best predictive linear combinations of the columns of **X** or, equivalently, RA is searching for the subspace of **X** where the projection of **Y** has the largest variance.

latent variable from **X**) is used, in a regression step, to predict **Y**. After the first latent variable has been used, its effect is partialled from **X** and **Y** and the procedure is re-iterated to find subsequent latent variables and loadings.

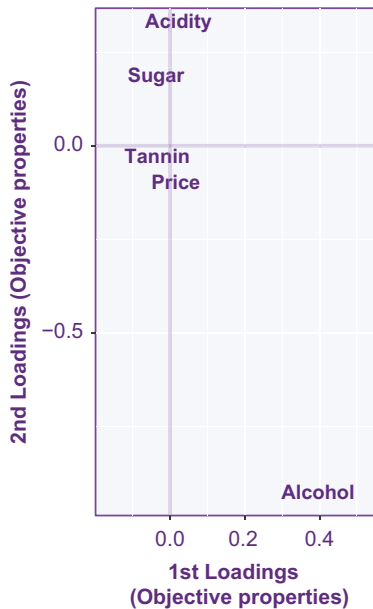
Partial Least Square Regression

Partial Least Square Regression (PLSR) – a technique tailored to cope with multicollinearity of the predictors in a regression framework – (see, e.g., Tenenhaus (1998); Abdi (2010) for reviews) starts just like IBA and extracts a first pair of latent variables with maximal covariance, then **f** (the

Particular Cases

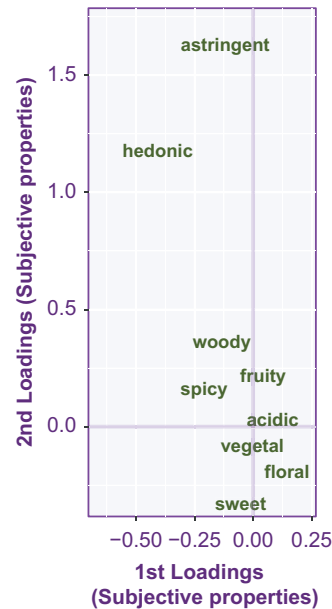
Noncentered CCA: Correspondence Analysis

An interesting particular case of *noncentered* CCA concerns the case of group matrices. In a group matrix, the rows represent observations



Canonical Correlation Analysis, Fig. 9 Loadings of the second LV versus the first LV for matrix X

(just like in plain CCA) and the columns represent a set of exclusive groups (i.e., an observation belongs to one and only one group). The group assigned to an observation has a value of 1 for the row representing this observation and all the other columns for this observation (representing the groups not assigned to this observation) will have a value of 0. When both X and Y are non-centered and nonnormalized group matrices, then the CCA of these matrices will give *correspondence analysis* – a technique developed to analyze contingency tables (see entry on correspondence analysis and, e.g., Greenacre (1984)). When X and Y are composed of the concatenation of several noncentered and nonnormalized group matrices, the CCA of these two tables will be equivalent to *partial least square correspondence analysis* (PLSCA (Beaton et al. 2016)) – a technique originally developed to analyze the information shared by two tables storing qualitative data. In the particular case when X is composed of the concatenation of several noncentered and nonnormalized group matrices, the CCA of



Canonical Correlation Analysis, Fig. 10 Loadings of the second LV versus the first LV for matrix Y

X with itself is equivalent to multiple correspondence analysis.

Some Other Particular Cases of CCA

CCA is a very general method and so a very large number of methods are particular cases of CCA (Abdi 2003). For example, when Y has only one column, CCA becomes (simple and multiple) linear regression. If X is a group matrix and Y stores one quantitative variable, CCA becomes analysis of variance. If Y is a group matrix, CCA becomes discriminant analysis. This versatility of CCA makes it of particular theoretical interest.

Key Applications

CCA and its derivatives – or variations thereof – are used when the analytic problem is to relate two data tables and this makes these techniques ubiquitous in almost any domains of inquiry from

marketing to brain imaging and network analysis (see Abdi et al., 2016, for examples).

Future Directions

CCA is still a domain of intense research with future developments likely to be concerned with multi-table extensions (e.g., Horst 1961; Tenenhaus et al. 2014), “robustification,” and sparsification (Witten et al. 2009). All these approaches will make CCA and its related techniques even more suitable for the analysis of very large data sets that are becoming prevalent in analytics.

Cross-References

- ▶ [Barycentric Discriminant Analysis](#)
- ▶ [Correspondence analysis](#)
- ▶ [Eigenvalues, Singular Value Decomposition](#)
- ▶ [Iterative Methods for Eigenvalues/Eigenvectors](#)
- ▶ [Least Squares](#)
- ▶ [Matrix Algebra, Basics of](#)
- ▶ [Matrix Decomposition](#)
- ▶ [Principal Component Analysis](#)
- ▶ [Regression Analysis](#)
- ▶ [Spectral Analysis](#)

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