A dual method of Carroll's generalized canonical correlation analysis

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We propose a dual method of Carroll's generalized canonical correlation analysis and we prove by means of the proposed criterion that the duality is formulated by exchanging the operators. It is an extension of Carroll's generalized canonical correlation analysis. The approach of analysis is illustrated on the basis of case study.

Keywords: Dual generalized canonical correlation analysis, data set partitioned in groups of individuals, principal component analysis.

1 Introduction

Hotelling (1936) proposed the first and oldest method called canonical correlation analysis. This method studies the relationships between two data matrices. Canonical correlation analysis focuses on the correlation between a linear combination of the variables in one set and a linear combination of the variables in another set. The idea is first to determine the pair of linear combinations having the largest correlation. Next, we determine the pair of linear combinations having the largest correlation among all pairs uncorrelated with the initially selected pair, and so on. Other developments of the canonical correlation analysis are in the research of Gittins (1985) and Saporta (2006).

A survey of the plethora of generalizations of canonical correlation analysis have been proposed for the analysis of the relationships with more than two sets of variables (e.g., Horst (1961), Carroll (1968), Kettenring (1971); see also Takane and Hwang (2002), Wold (1982, 1985), Gifi (1990), Takane and Oshima-Takane (2002), Dahl and Næs (2006), Hanafi and Kiers (2006)). However, we will restrict ourselves to the Carroll's (1968) generalization.

Currently, in the context where the set of variables is observed on different groups of individuals, this problem has been studied in many scientific articles. If one expects the structure of each of the data blocks to be different, standard principal component analysis (PCA) (Jolliffe (2002), Pearson (1901)) can be performed on each data block. Moreover, one can carry out the simultaneous processing of all groups of variables. First, methods that are similar to PCA. Several methods combine the covariance matrices or the correlation matrices related to the various groups. The goal of these methods is to redistribute the explained variance by rotation. Krzanowski (1984) proposed to carry out a multigroup PCA by diagonalizing the within group covariance matrix. This problem has been reworked and developed into a succession of PCA by Eslami, Qannari, Kohler and Bougeard (2013). In this context, we can cite the common principal component analysis (Flury (1984)), simultaneous component analysis methods (Kiers and Ten Berge (1989, 1994), Timmerman and Kiers (2003), De Roover, Ceulemans and Timmerman (2012)).

In practice, when we have a group of variables, the cloud of the individuals and the cloud of the variables are two representations of the same group: one across the rows and the other across the columns. Very strong relations called duality link these two clouds. Thus, there is an equivalence between multigroup data analysis methods and multiblock data analysis methods. In these conditions, several multigroup data analysis methods, such as the dual STATIS (Lavit (1988); Lavit, Escoufier, Sabatier and Traissac (1994)), the dual multiple factor analysis (L, Husson and Pags (2010)), can be seen as dual methods of multiblock data analyses.

Moreover, there are similar methods to the canonical correlation analysis among multigroup data analyses. We can cite: Between groups comparison of principal components (Krzanowski (1979)) and Regularized generalized canonical correlation analysis for multiblock or multigroup data analysis (Takane, Hwang and Abdi (2008), Tenenhaus and Tenenhaus (2017)).

However, in the context where the set of variables is observed on different groups of individuals, the generalization of canonical correlation analysis (GCCA) according to Carroll (1968) has never been discussed. In this paper, a version of GCCA called DGCCA (Dual generalized canonical correlation analysis), which can be applied to multiblock and multigroup, is discribed. We prove by means of the criterion that the duality is formulated by exchanging the covariance operator into scalar product. This criterion can be seen as a PCA in which the influence of the variables is stable.

This paper is organized as follows: in Section 2, we will describe the canonical correlation analysis proposed by Hotelling (1936) and extended by Carroll (1968). In section 3, by using the criterion proposed by Carroll, we will propose the dual generalized canonical correlation analysis (section 3.1). Next, we also show that the dual generalized canonical correlation analysis can be reduced to the dual canonical correlation analysis (section 3.2) in the case of two matrices. Finally, in section 4, the experimental design is described and the obtained results are analyzed.

2 Materials and methods

2.1 Generalized canonical correlation analysis

We shall be interested in measures of association between two matrices. The first matrix X_1, of p columns, is summarized by the $(n \times 1)$ canonical variate $X_1 u_1$. The second matrix X_2, of q columns, is summarized by the $(n \times 1)$ canonical variate $X_2 u_2$. Specifically, we define canonical correlation analysis as the following optimization problem:

$$\text{Maximize} \qquad corr(X_1 u_1, X_2 u_2) \tag{1}$$

$$\text{subject to the constraints} \quad var(X_1 u_1) = var(X_2 u_2) = 1$$

The first pair of canonical variates is the pair of linear combinations $(X_1 u_1^1, X_2 u_2^1)$ having unit variances, which maximize the correlation (1); The second pair of canonical variates is the pair of linear combinations $(X_1 u_1^2, X_2 u_2^2)$ having unit variances, which maximize the correlation (1) among all choices that are uncorrelated with the first pair of canonical variates. One may continue the search for canonical variates until all solutions are found.

To generalize the canonical correlation analysis of two sets of variables to K sets of variables, let X be a matrix $X = [X_1, \ldots, X_K]$ having n rows and $p = \sum_{i=1}^{K} p_i$ columns, partitioned in K submatrices X_i. Each $n \times p_i$ $(n > p_i)$ data matrix X_i represents a set of p_i centered and standardized variables observed on a set of n individuals. Let E_i $(i = 1, \ldots, K)$ denote column spaces of X_i. Let P_i be the orthogonal projector onto the column space E_i of X_i, $P_i = X_i(X_i' X_i)^{-1} X_i'$.

We only consider in this paper the generalization developed by Carroll (1968) which consists of the following optimization problem:

$$\text{Maximize} \qquad \frac{1}{N} \sum_{i=1}^{K} corr^2(z, X_i u_i) \tag{2}$$

$$\text{subject to the constraint} \quad z'z = 1$$

The principle of the generalized canonical correlation analysis is first to investigate the variables related to the set of the groups. These variables which summarize the general trends of the groups are called general variables. Futhermore, a general variable being obtained, we seek in each group a linear combination of variables related to this general variable. These linear combinations called canonical variates are the representations of the general variables in groups.

One of the advantages of this approach is to obtain the solution noniteratively (Kroonenberg (2008)). Another advantage of this approach is that it is not necessary to define a link measurement between two groups of variables but between a variable and a group (Escofier and Pags (2008)). The measurement used by Carroll (1968) is the square of the multiple correlation coefficient. Finally, this approach has the advantage of being probably the most simple and the richest of interpretations, because it easily connects to all the other methods of data analysis.

By definition, the multiple correlation coefficient between a variable and a group of variables X_i is the correlation coefficient between z and the linear combination of the variables of the group X_i most correlated with z. Geometrically, this linear combination is the orthogonal projection $P_i z$ of z onto the column space E_i of X_i.

The relationship between the correlation coefficients and the variable z follows from the special structure of the matrix $\sum_{i=1}^{K} P_i$. In other words, the generalized canonical correlation analysis verifies the following stationary equation:

$$\frac{1}{N}\sum_{i=1}^{K} P_i z = \rho z \tag{3}$$

The solution of the generalized canonical correlation analysis shows that it can be obtained from the principal component analysis (Gifi (1990), Saporta (2006)). Thus, by setting $\Sigma_i = X_i' X_i$, the solution of GCCA verifies the following stationary equation:

$$XDX'z = \rho z \tag{4}$$

where D is a block diagonal matrix formed from Σ_i^{-1} as the ith diagonal block.

The GCCA is similar to a PCA in which each column space E_i of X_i is associated with the matrix Σ_i^{-1}.

In this section we will give some details of a solution to the dual generalized canonical correlation analysis.

2.2 Dual generalized canonical correlation analysis

We now consider a matrix $X = [X_1'|\cdots|X_K']'$ having $n = \sum_{i=1}^{K} n_i$ rows and p columns, partitioned in K submatrices X_i of order $(n_i \times p)$ and row spaces E_i $(i = 1, \ldots, K)$ of X_i. Each data matrix X_i represents a set of p centered and standardized variables observed on a set of n_i individuals. Let J_i be the orthogonal projector onto the row space E_i of X_i, $J_i = X_i'(X_i X_i')^- X_i$, where A^- is a g-inverse of A.

2.2.1 Definition of Dual generalized canonical correlation analysis

In the first step, the solution of the dual generalized canonical correlation analysis is a loading vector u and specific coefficients $t_i = X_i' a_i$ (a_i being a vector to be determined of order $(n_i \times 1)$) associated with data matrices X_i $(i = 1, \ldots, K)$.

In our case, as in many similar situations, we define a mean-squared loss function. The core optimization problem considered in this paper is defined as follows:

$$\text{Minimize} \qquad g(u) = \frac{1}{N}\sum_{i=1}^{K} ||u - J_i u||^2 \tag{5}$$

$$\text{subject to the constraints} \quad ||u|| = ||t_i|| = 1.$$

The loading vector is common to all matrices and its projection onto the subspace E_i is the specific coefficient $t_i = J_i u$. To convert the minimization problem into a maximization problem we rewrite (5) and manipulate the various terms. We obtain the following maximization problem:

$$\text{Maximize} \qquad h(u) = \frac{1}{N}\sum_{i=1}^{K} \langle u | J_i u \rangle = \frac{1}{N}\sum_{i=1}^{K} u' J_i u \tag{6}$$

$$\text{subject to the constraints} \quad ||u|| = ||t_i|| = 1.$$

From this problem, we can incorporate the constraint in the maximization problem by using Lagrange multiplier λ and obtain $\tilde{h}$,

$$\tilde{h}(u, \lambda) = h(u) - \lambda(u'u - 1) \tag{7}$$

The maximum of h follows from the requirement that the first order partial derivatives of $\tilde{h}$ are simultaneously zero at the maximum of h and that the Hessian is negative. We will state here the exact nature of the solution as proposition.

Proposition 2.1 *For $J_i u = t_i$, we obtain the following result:*

$$\frac{1}{N}\sum_{i=1}^{K} J_i u = \lambda u \tag{8}$$

Proof 3.1: Differentiating with respect to u and λ, and setting all the derivatives equal to zero, we obtain the following set of equations which have to be solved simultaneously for u and λ. Thus,

$$\begin{aligned} \frac{1}{N}\sum_{i=1}^{K} J_i u &= \lambda u \\ u'u &= 1 \end{aligned}$$

It can be easily shown that for $J_i u = t_i$, the solution u verifies the stationary equation where u is a eigenvector of the matrix $\frac{1}{N}\sum_{i=1}^{K} J_i$ related to the largest eigenvalue λ. By replacing J_i in $J_i u = t_i$ and taking into account of $t_i = X_i' a_i$, we obtain $a_i = (X_i X_i')^{-} X_i u$. The partial components are obtained by setting $\xi_i = X_i u$.

Moreover, as the projectors J_i are symmetric and idempotent, it follows that $h(u) = \frac{1}{N}\sum_{i=1}^{K} ||J_i u||^2$. It seems that the dual generalized canonical correlation analysis (DGCCA) is similar to principal component analysis (PCA)(see proposition 3.2). The components are determined using the same loading vector u and the explained variance can be redistributed by rotation. It can be easily shown that the vector u which maximizes this average inertia is obtained by the eigenvector of $\frac{1}{N}\sum_{i=1}^{K} J_i$ related to the eigenvalue $\lambda = \frac{1}{N}\sum_{i=1}^{K} ||J_i u||^2$.

That is, after finding a first axis, this column is fixed and the second column is found in the residual space, by replacing X_i by $X_i(I_p - uu')$ and proceeding in the same way as for the first step. Other loading vectors can be obtained by repeating the procedure. This procedure allows to construct the orthonormal basis. We can remark that the global components $\xi^s = Xu^s$ ($s = 1\ldots, A$, where A is the rank of the matrix X) are orthogonal. The following proposition establishes that the dual generalized canonical correlation analysis is a PCA.

Proposition 2.2 *For $W_i = X_i X_i'$, the dual generalized canonical correlation analysis is a PCA and verifies the following stationary equations:*

$$X' D^- X u = \lambda u \tag{9}$$

$$X X' D^- \xi = \lambda \xi \tag{10}$$

where D^- is a block diagonal matrix formed from W_i^- as the ith diagonal block.

Proof 3.2: Indeed, as we have indicated, the same components may be determined by the PCA of the matrix X. One only has to consider X as a matrix having $n = \sum_{i=1}^{K} n_i$ rows and p columns and $J_i = X_i'(X_i X_i')^{-} X_i$, we then set $W_i = X_i X_i'$ as the matrix of scalar products between observations in the row space of X_i and Λ^- the block-diagonal matrix formed from W_i^-. We obtain $\sum_{i=1}^{K} J_i = \sum_{i=1}^{K} X_i' W_i^- X_i = X'\Lambda^- X$. The stationary equation (8) becomes (11)

$$\frac{1}{N} X'\Lambda^- X u = \lambda u. \tag{11}$$

By setting $D^- = \frac{1}{N}\Lambda^-$ and by premultiplying (11) by X, it follows

$$X X' D^- \xi = \lambda \xi$$

$$X' D^- X u = \lambda u.$$

We then recognize the eigen equations yielding principal components and factor axes in PCA of X.

From the above,we conclude that the criterion of DGCCA is a PCA in which the duality is formulated by exchanging the covariance matrix Σ_i into scalar product matrix W_i. So, It is about substituting the block diagonal matrix D formed from Σ_i^{-1} by the block-diagonal matrix Λ^- formed from W_i^-.

Geometrically, each specific coefficient t_i associated with different matrices is the orthogonal projection $J_i u$ of u onto the subspaces E_i spanned by the rows of X_i. Thus, the multiple correlation coefficient is the cosine of the angle θ_i between the loading vector u and its projection $J_i u$ onto E_i. Since u and $J_i u$ are normalized, we then have:

$$\cos^2\theta_i = \langle u | J_i u\rangle.$$

As $u^{s'}(u^{s-1}, \ldots, u^1) = 0$, we obtain:

$$\sum_{i=1}^{K} \cos^2\theta_i = \sum_{i=1}^{K} \langle u^s | J_i u^s\rangle = \langle u^s | \sum_{i=1}^{K} J_i u^s\rangle.$$

We achieve the same conclusion: the operator $\sum_{i=1}^{K} J_i$ being a sum of the orthogonal projection operators, It is symmetric, diagonalizable and the eigenvectors are orthonormal.

2.2.2 Dual canonical correlation analysis

We shall be interested in the measures of association between two data matrices. Let E_1 and E_2 be the row spaces of X_1 and X_2. We also introduce for each matrix, unit vectors $t_1 = X_1' a_1$ and $t_2 = X_2' a_2$ onto E_1 and E_2 repectively. The two vectors are as close as possible. Let J_1 and J_2 be orthogonal projections onto E_1 and E_2 defined by: $J_1 = X_1'(X_1 X_1')^{-} X_1$ and $J_2 = X_2'(X_2 X_2')^{-} X_2$ where A^- is a g-inverse of A. Let $W_1 = X_1 X_1'$ and $W_2 = X_2 X_2'$ be scalar product matrices. Let W_{12} be the scalar product matrix of the individuals inter-data matrices and W_{21} its transpose.

The dual canonical correlation analysis (DCCA) problem consists of optimizing the following squared distance from $t_1 = J_1 u$ and $t_2 = J_2 u$:

$$\text{Minimize} \qquad k(a_1, a_2) = ||t_1 - t_2||^2 \tag{12}$$
$$\text{subject to the constraints} \quad ||t_1|| = ||t_2|| = 1.$$

This problem is equivalent to optimize the following criterion:

$$\text{Maximize} \qquad k_1(a_1, a_2) = a_1 W_{12} a_2 \tag{13}$$
$$\text{subject to the constraints} \quad a_1 W_1 a_1 = a_2 W_2 a_2 = 1$$

We define dual canonical correlation (DCCA) as the optimization problem which consists of measuring the proximity of the individuals between the groups X_1 and X_2. The Lagrangian function of optimization problem (8) is then considered:

$$\tilde{k_1}(a_1, a_2, \lambda_1, \lambda_2) = a_1 W_{12} a_2 - \frac{\lambda_1}{2}(a_1 W_1 a_1 - 1) - \frac{\lambda_2}{2}(a_2 W_2 a_2 - 1) \tag{14}$$

where λ_1 and λ_2 are the Lagrange multipliers associated with the constaints. Canceling the derivatives of the Lagrangian function with respect to a_1, a_2, λ_1 and λ_2, we obtain using the stationary equations:

- a_1 is the eigenvector of the matrix $W_1^- W_{12} W_2^- W_{21}$ associated with the largest eigenvalue λ_1^2,
- a_2 is the eigenvector of the matrix $W_2^- W_{21} W_1^- W_{12}$ associated with the largest eigenvalue λ_1^2.

The eigenvectors t_1 and t_2 are associated with the same eigenvalues. Thus, in DCCA, we also get:

- t_1 is the eigenvector of the matrix $J_1 J_2$ associated with the largest eigenvalue λ_1^2,
- t_2 is the eigenvector of the matrix $J_2 J_1$ associated with the largest eigenvalue λ_1^2.

Remarks 2.1 (See proof in the Appendix)

1. *The dual generalized canonical correlation analysis generalizes the dual canonical correlation analysis.*
2. *The loading vector u is the principal factor according to normalized PCA of the vectors t_i.*
3. *The mean (sum) of the specific coefficients t_i and u are proportional.*

3 Results

We present the results of the dual generalized canonical correlation analysis and we repeat part of the multigroup PCA of Eslami, Qannari, Kohler and Bougeard (2013). The data set is the one used by Cortez, Cerdeira, Almeida and Reis (2009) and by Eslami, Qannari, Kohler and Bougeard (2013). The study focuses on Portuguese wines. Specifically, we reanalyze matrices of eleven physicochemical variables observed on 4898 individuals for the white wines and 1599 individuals for the red wines. To eliminate the differences in variable means and variances, the data are centered and standardized per data matrix.

Regarding the graphical representation, the physicochemical variables are as follows:

Fixac=fixed acidity, Volac=volatile acidity, Citac=citric acid, Resug=residual sugar, Chlor=chlorides, Fredi=free sulfur dioxide, Totdi=total sulfur dioxide, Densi=density, pH, Sulph=sulphates, Alcoh=alcohol.

The goal of the dual generalized canonical correlation analysis is to help discover how the relationships vary in the experimental setup. In Table 1 below, we report the percentages of explained variances for first four principal components and global components obtained from the dual generalized canonical correlation analysis. Table 2 give the analogous results for the multigroup PCA.

Table 1: The percentages of the explained variances of DGCCA

Group	Dim1	Dim2	Dim3	Dim4
Red wines	28.61	13.74	11.69	9.30
White wines	21.96	21.51	10.44	10.41
Global component	44.02	19.17	11.94	8.29

Table 2: The percentages of the explained variances of multigroup PCA

Group	Dim1	Dim2	Dim3	Dim4
Red wines	29.19	14.08	11.21	9.28
White wines	23.36	21.58	13.46	11.12
Global component	27.25	15.91	11.61	9.75

Figure 1 shows the representation of the variables on the first two loading vectors. The proportion of total variance accounted for the first principal component is 44.02%. The first principal component which explains 44.02% of the total variance, has an interesting subject-matter interpretation. The first principal component opposes the alcohol concentration to the sugar concentration and the density. Moreover, this component is correlated with sulphates and chlorides. This corresponds to the fermentation where some variables can be increased or decreased in the production process.

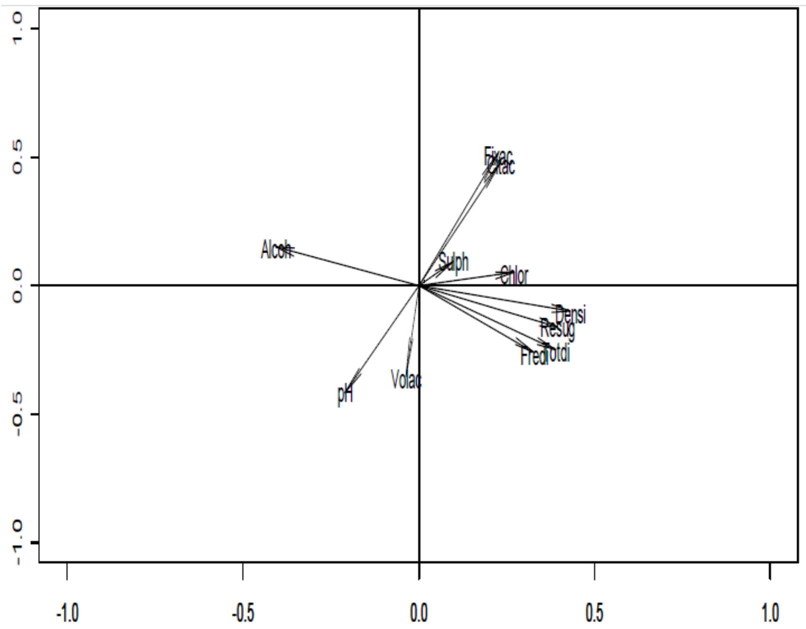

Figure 1: Map of the columns on the first two loading vectors of DGCCA

The second axis explains 19.17% of the total variance. The first two principal components, collectively, explain 63.19% of the total variance, which is a very well result. The second axis represents 19.17% of the total variance and shows an opposition between the acid measurements and the pH.

For each of the two analyses, the eigenvalues of DGCCA are superior to the eigenvalues of multigroup PCA. The results of the DGCCA and the multigroup PCA are very little different.

4 Concluding Remarks

In this paper, the duality between generalized canonical correlation analysis and its dual method is clearly defined. Generalized canonical correlation analysis uses the covariance operator, while dual generalized canonical correlation analysis uses the scalar product operator. The main aim of generalized canonical correlation analysis is to investigate the relationships between blocks, while the main aim of dual generalized canonical correlation analysis is to investigate the relationships among variables within the various groups. the PCA can be considered for both multiblock and multigroup data. The dual generalized canonical correlation analysis benefits the same advantages that the generalized canonical correlation analysis according to Carroll. We have shown in this paper that due to their higher flexibility and properties, it can be considered a straightforward extension of the PCA to multigroup PCA which facilitates the interpretation of results. The DGCCA criterion opens several ways of research in particular to find variables that discriminate the groups of variables. Moreover, if the number of individuals is much smaller than the number of variables, this method may exhibit instability due to ill-conditioned scalar product matrix. Under these conditions, a regularization of the method may be useful as in the case of generalized canonical correlation analysis (Tenenhaus et al. (2011), Takane, Hwang and Abdi (2008)).

Appendix A. Proofs of the remarks

Proof of 1. The dual generalized canonical correlation analysis generalizes the dual canonical correlation analysis.

Indeed, the normalization constraints are the same as those of the dual canonical correlation analysis. To minimize $||u - J_1 u||^2 + ||u - J_2 u||^2$ subject to the normalization constraints over u, t_1 and t_2 is equivalent to minimize $||J_1 u - J_2 u||^2$.

$$\begin{aligned} ||u - J_1 u||^2 + ||u - J_2 u||^2 &= \langle J_1 u | u \rangle + \langle u | J_2 u \rangle \\ &= \langle J_1 u | J_2 u \rangle \\ &= ||J_1 u - J_2 u||^2 \end{aligned} \tag{15}$$

Proof of 2. The loading vector u is the principal factor according to normalized PCA of the vectors t_i.

In fact the specific coefficients being given, u is the loading vector that yields maximum $\frac{1}{N}\sum_{i=1}^{K} ||u - J_i u||^2$, then by definition the principal factor of the specific coefficients t_i.

Proof of 3. The mean (sum) of the t_i and u are proportional.

Indeed, The stationary equation (8) shows that the only possible proportionality constant is λ. Since

$$\frac{1}{N}\sum_{i=1}^{K} t_i = \frac{1}{N}\sum_{i=1}^{K} J_i u = \lambda u \tag{16}$$

λ being the largest eigenvalue of the mean (sum) of J_i.

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