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Rotation in Multiple Correspondence Analysis: a planar rotation iterative procedure

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Rotation en Analyse des Correspondances Multiples : une procédure de rotation planaire itérative

Résumé

L'Analyse des Correspondance Multiples (ACM) est une méthode d'analyse multidimensionnelle bien connue pour la description d'un jeu de données qualitatives. Comme en Analyse en Composantes Principales (ACP) ou en Analyse en Facteurs, la rotation peut être utilisée pour simplifier la lecture des résultats numériques. L'idée est d'appliquer une matrice de rotation à la matrice des composantes principales afin de voir se former des groupes de variables et interpréter plus facilement les composantes principales. En ACP, le critère le plus connu est probablement le critère varimax proposé par Kaiser (1958). D'autre part, Kiers (1991) s'est intéressé à ce problème dans le cadre de la méthode PCAMIX qu'il a développée pour l'analyse de données mixtes (qualitatives et quantitatives). Cette méthode inclut ainsi comme cas particuliers l'ACP et l'ACM. Il propose un critère de rotation qui dans le cas purement qualitatif est basé sur les rapports de corrélation entre les variables qualitatives et les composantes principales. Il utilise l'algorithme de De Leeuw et Pruzansky (1978) pour optimiser ce critère. Dans cet article, nous utilisons ce même critère de rotation et nous définissons, dans le cas particulier de deux dimensions (rotation planaire), l'expression analytique de l'angle optimal de rotation. Dans le cas de plus de deux dimensions, nous utilisons la procédure de rotations successives planaires, proposée par Kaiser (1958) pour la rotation en ACP. Une étude sur simulations permet de vérifier l'exactitude de la solution analytique et de visualiser l'impact de la rotation. Enfin, une étude de cas réelle illustre les intérêts potentiels de la rotation en ACM.

Mots-clés : données qualitatives, analyse des correspondances multiples, rapport de corrélation, rotation, critère varimax

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Abstract

Multiple Correspondence Analysis (MCA) is a well-known multivariate method for statistical description of categorical data (see for instance Greenacre and Blasius, 2006). Similarly to what is done in Principal Component Analysis (PCA) and Factor Analysis, the MCA solution can be rotated to increase the components simplicity. The idea behind a rotation is to find subsets of variables which coincide more clearly with the rotated components. This implies that maximizing components simplicity can help in factor interpretation and in variables clustering. In PCA, the probably most famous rotation criterion is the varimax one introduced by Kaiser (1958). Besides, Kiers (1991) proposed a rotation criterion in his method named PCAMIX developed for the analysis of both numerical and categorical data, and including PCA and MCA as special cases. In case of only categorical data, this criterion is a varimax-based one relying on the correlation ratio between the categorical variables and the MCA numerical components. The optimization of this criterion is then reached by the algorithm of De Leeuw and Pruzansky (1978). In this paper, we give the analytic expression of the optimal angle of planar rotation for this criterion. If more than two principal components are to be retained, similarly to what is done by Kaiser (1958) for PCA, this planar solution is computed in a practical algorithm applying successive pairwise planar rotations for optimizing the rotation criterion. A simulation study is used to illustrate the analytic expression of the angle for planar rotation. The proposed procedure is also applied on a real data set to show the possible benefits of using rotation in MCA.

Keywords: categorical data, multiple correspondence analysis, correlation ratio, rotation, varimax criterion

JEL : C49 ; C69

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Rotation in Multiple Correspondence Analysis: a planar rotation iterative procedure

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Abstract

Multiple Correspondence Analysis (MCA) is a well-known multivariate method for statistical description of categorical data. Similarly to what is done in Principal Component Analysis (PCA) and Factor Analysis, the MCA solution can be rotated to increase the components simplicity. The idea behind a rotation is to find subsets of variables which coincide more clearly with the rotated components. This implies that maximizing components simplicity can help in factor interpretation and in variables clustering. In this paper, we propose a two-dimensional analytic solution for rotation in MCA. Similarly to what is done by Kaiser (1958) for PCA, this planar solution is computed in a practical algorithm applying successive pairwise planar rotations for optimizing the rotation criterion. This criterion is a varimax-based one relying on the correlation ratio between the categorical variables and the MCA components. A simulation study is used to illustrate the proposed solution. An application on a real data set shows the possible benefits of using rotation in MCA.

Keywords: categorical data, multiple correspondence analysis, correlation ratio, rotation.

1 Introduction

Multiple Correspondence Analysis (MCA) is the french name (Benzécri, 1973; Lebart, Morineau and Warwick, 1984) for a multivariate quantification method of categorical data. This method has been proposed by many different authors under various names. Among others we can mention the Dutch Homeneity Analysis (Gifi, 1990), the Japanese Quantification Method (Hayashi, 1954), the Canadian Dual Scaling (Nishisato, 1980, 1994). All these methods with different theoretical foundations lead usually to equivalent solutions (Tenenhaus and Young, 1985). A recent survey of various approaches from different statistical "schools" can be found in Greenacre and Blasius (2006).

In the present paper, our treatment and interpretation of MCA resemble that of PCA (Benzécri, 1973; Greenacre, 1984: chapter 3). Indeed, MCA is concerned with observations of p categorical variables for each n samples and may be viewed as a form of PCA applicable to categorical variables rather than quantitative variables. However, special emphasis will be placed on the fact that, as in Correspondence Analysis (CA) (Greenacre, 1984: chapter 2 and appendix), MCA solutions are neatly encapsulated in the Singular Value Decomposition (SVD) of a suitably transformed matrix. More precisely, the relationship between MCA and the lower rank approximation approach of biplot (Greenacre, 1993 or Gower and Hand, 1996) provides the mathematical scaffolding for applying rotation methods in MCA.

In PCA and Factor Analysis (FA), objective criteria have been proposed for the attainment of simple structure. The varimax criterion introduced by Kaiser (1958) is by far the most commonly used criterion for rotation in PCA. This criterion aims at maximizing the sum over the columns of the squared elements of the loading matrix. The loading matrix plays indeed a major part in the interpretation of the results since it contains the correlations between the variables and the principal components. The idea is to get components for which the interpretation is easier, that is to rotate the loading matrix and the standardized principal components such that groups of variables appear, having high loadings on the same component, moderate on a few components and negligible on the remaining ones. Because the lower-rank approach in PCA gives the freedom for orthogonal rotation, the only consequence is that the percentage of variance explained is redistributed along newly rotated axes, while still conserving the variance explained by the solution as a whole. In practice, defining the best orthogonal rotation matrix sums up to a constrained optimization problem. When a solution requires only two dimensions the rotation occurs in a plane and the rotation matrix can be written according to a rotation angle θ leading to an unconstrained real optimization problem. When the interpretation of three or more dimensions is required, the analytic expression of θ optimizing the Varimax criterion is used by Kaiser (1958) in a practical algorithm applying successive pairwise planar rotations. Several other algorithms for the maximization of the Varimax criterion have since been proposed in literature: see for instance Neudecker, (1981); Sherin (1966) or ten Berge (1984).

As has already been pointed, MCA and thus CA too, is a particular case of weighted PCA. Despite this close relationship with a method in which rotation is quite common, rotation in CA has not received much attention: Van de Velden and Kiers (2003, 2005) and Greenacre (2006) explicitly considered rotation in CA.

Their results, however, do not carry out over to rotation in MCA. Adachi (2004) considered oblique rotation in MCA. Oblique and orthogonal rotation involves the same problem of maximizing a simplicity criterion. Only the imposed constraints differ. Since fewer constraints are imposed in oblique rotation, it is generally possible to obtain simpler solution than in orthogonal rotation (Browne, 2001). Despite this advantage, orthogonal rotations are commonly used in practice. Indeed, the orthogonality leads to direct interpretation of the rotated axes: the orthogonally rotated loadings can be directly interpreted as correlations between the variables and the rotated standardized principal components and graphical representations remain possible. Kiers (1991) considered orthogonal rotation in PCAMIX. This method, developed for the analysis of a mixture of categorical and numerical variables, includes PCA and MCA as special cases. The several rotation techniques proposed for simple structure in PCAMIX solution can then be applied to MCA solutions. In PCA, the rotation criteria are defined on the correlations between variables and principal components. For qualitative variables, however, the correlation can not be used and another coefficient has to be chosen to express the link between a categorical variable and a (quantitative) component. Kiers (1991) used for rotation in PCAMIX, and then in MCA, the discrimination measure (Gifi, 1990) defined as the contribution of a component to the inertia of a variable that is accounted for. This measure can be interpreted as the squared correlation between a variable optimally quantified and a principal component (Gifi, 1990, p.96), or alternatively, as the well-known correlation ratio. The idea of simple structure in MCA is to rotate the component coordinates such that groups of categorical variables appear, having high correlation ratio on the same component, moderate on a few components and negligible on the remaining ones. The research of simple structure in MCA can then be operated by applying orthogonal rotation criteria to the correlation ratio matrix. Kiers (1991) gave in this framework a matrix formulation of the orthomax criterion (including varimax) which permits interpreting this rotation problem as a simultaneous diagonalization of a set of symmetric matrices (ten Berge, 1984), and proposed to use the algorithm of de Leeuw and Pruzansky (1978) for that simultaneous diagonalization.

The main contribution of this paper is the definition of the analytic expression of the angle θ for orthogonal planar rotation in MCA, optimizing the correlation ratio based Varimax criterion. The relevance of finding an analytic solution for two dimensional MCA is first that this solution can be used in divisive clustering of categorical data, which was our first motivation for this work. Moreover, this planar solution can be used, as the planar solution proposed by Kaiser (1958), in a practical algorithm applying successive pairwise planar rotations for optimizing the rotation criterion in more than two dimensions. This procedure is an alternative to that proposed by Kiers (1991). We also try to give in this paper a pedagogic and relatively detailed presentation of the problem of rotation in MCA, which has not been extensively studied yet. Therefore, we remind the relations between the french geometric presentation of PCA and MCA, and the matrix lower-rank approximation approach of biplots.

In Section 2 we recall the principles of MCA. In Section 3 we consider the rotation problem to obtain simple structure in MCA and we give the expression of the analytic solution for two-dimensional rotation. A simulated example is used to illustrate planar rotation. A real data application is treated in Section 4 to show the potential benefits of using rotation in MCA. Finally concluding remarks are given in Section 5.

2 Recall on multiple correspondence analysis

In this section the theory of MCA is summarized in order to define the terms and notation for the later sections. The basic data we start with are n observations on p categorical variables. Suppose variable j can assume q_j different values. We can code the data using indicator matrices (also known as dummies). Indicator matrix $\mathbf{G}_j$ is $n \times q_j$. It consists of zeroes and ones, and it has exactly one element equal to one in each row, indicating in which category of variable j object i belongs. By concatenating the $\mathbf{G}_j$ we obtain the $n \times q$ matrix $\mathbf{G}$, with q the sum of the q_j.

MCA is defined in this paper as the application of simple CA to the indicator matrix $\mathbf{G}$. Hence CA, and then MCA too, are defined as the application of weighted PCA to the indicator matrix $\mathbf{G}$ (Benzécri, 1973; Greenacre, 1984: chapter 3). More precisely, $\mathbf{G}$ is divided by its grand total np to obtain the so-called "correspondence matrix" $\mathbf{F} = \frac{1}{np}\mathbf{G}$, so that $\mathbf{1}_n^t\mathbf{F}\mathbf{1}_q = 1$, where, generically, $\mathbf{1}_i$ is an $i \times 1$ vector of ones. Furthermore, the row and column marginals define respectively the vectors $\mathbf{r} = \mathbf{F}\mathbf{1}_q$ and $\mathbf{c} = \mathbf{F}^t\mathbf{1}_n$, that is the vectors of row and column masses. Let $\mathbf{D}_r = \mathrm{diag}(\mathbf{r})$ and $\mathbf{D}_c = \mathrm{diag}(\mathbf{c})$ be the diagonal matrices of these masses. In this particular case, the ith element of $\mathbf{r}$ is $f_{i.} = \frac{1}{n}$ and the sth element of $\mathbf{c}$ is $f_{.s} = \frac{n_s}{np}$ where n_s is the frequency of category s.

Weighted PCA of the row profiles. The objects are described here by the row profiles which are points in $\mathbb{R}^q$ calculated by dividing the rows of $\mathbf{F}$ by their row marginals. They are weighted by the row masses in $\mathbf{r}$ and their centroid (weighted average) turns out to be exactly the vector of marginal column totals $\mathbf{c}^t$. MCA is then defined as the application of PCA to the centered matrix $\mathbf{D}_r^{-1}(\mathbf{F}-\mathbf{rc}^t)$ with distances between profiles measured by the chi-squared metric defined by $\mathbf{D}_c^{-1}$. From a geometrical point of view, this weighted PCA searches for $k \leq \text{rank}(\mathbf{F})$ orthogonal principal axes such that for each principal axe, the variance of the $\mathbf{D}_c^{-1}$-projections of the n profiles is maximal. The coordinates of the n projected row profiles on these principal axes are called *row principal coordinates*. Note that row (resp. coordinates) is sometimes replaced by object (resp. scores). The $n \times k$ matrix $\mathbf{X}$ of row principal coordinates is defined by:

$$\mathbf{X} = \mathbf{D}_r^{-1/2}\widetilde{\mathbf{F}}\mathbf{V}_k, \tag{1}$$

where $\widetilde{\mathbf{F}} = \mathbf{D}_r^{-1/2}(\mathbf{F}-\mathbf{rc}^t)\mathbf{D}_c^{-1/2}$ and $\mathbf{V}_k$ is the $q \times k$ matrix of eigenvectors corresponding to the k largest eigenvalues $\lambda_1, ..., \lambda_k$ of the matrix $\widetilde{\mathbf{F}}^t\widetilde{\mathbf{F}}$ (see Appendix 1 for a short recall on this wellknown result). Similarly to what is done in PCA, these projected row profiles can be plotted, for visualization and interpretation, in the different planes defined by these principal axes called *row principal planes*.

Weighted PCA of the column profiles. The categories are described here by the column profiles which are points in $\mathbb{R}^n$ calculated by dividing the columns of $\mathbf{F}$ by their column marginals. The dual analysis of columns profiles can be defined simply by interchanging rows with columns and all associated entities, i.e. transposing the matrix $\mathbf{F}$ and repeating all the above. The metrics used to define the principal axes in the weighted PCA of the centered profiles matrix $\mathbf{D}_c^{-1/2}(\mathbf{F}-\mathbf{rc}^t)^t$ are $\mathbf{D}_c$ on $\mathbb{R}^q$ and $\mathbf{D}_r^{-1}$ on $\mathbb{R}^n$. The coordinates of the q projected column profiles on these principal axes are called *column principal coordinates*. Note that column (resp. coordinates) is sometimes replaced by category (resp. scores). The $q \times k$ matrix $\mathbf{Y}$ of columns principal coordinates is defined by:

$$\mathbf{Y} = \mathbf{D}_c^{-1/2}\widetilde{\mathbf{F}}^t\mathbf{U}_k, \tag{2}$$

where $\mathbf{U}_k$ is the $n \times k$ matrix of eigenvectors corresponding to the k largest eigenvalues $\lambda_1, ..., \lambda_k$ of the matrix $\widetilde{\mathbf{F}}\widetilde{\mathbf{F}}^t$. These projected column profiles can be plotted, for visualization and interpretation, in the planes defined by these principal axes called *column principal planes*.

Use of SVD. The computational algorithm to obtain the principal coordinates of the row and column profiles with respect to principal axes is obtained with SVD:

$$\widetilde{\mathbf{F}} = \mathbf{U}\Lambda\mathbf{V}^t \tag{3}$$

where $\mathbf{U}^t\mathbf{U} = \mathbf{V}^t\mathbf{V} = \mathbb{I}_r$, Λ is the diagonal matrix with singular values on the diagonal, in weakly descending order, and r is the rank of $\widetilde{\mathbf{F}}$. It follows indeed from (3) that expression (1) (resp. (2)) of the row (resp. column) principal coordinates matrix can be rewritten:

$$\mathbf{X} = \mathbf{D}_r^{-1/2}\mathbf{U}_k\Lambda_k \text{ (resp. } \mathbf{Y} = \mathbf{D}_c^{-1/2}\mathbf{V}_k\Lambda_k). \tag{4}$$

The barycentric property. From (3) and (4), we obtain:

$$\mathbf{Y} = \mathbf{D}_c^{-1}(\mathbf{F} - \mathbf{r}\mathbf{c}^t)^t\mathbf{X}^* \tag{5}$$

where $\mathbf{X}^* = \mathbf{D}_r^{-1/2}\mathbf{U}_k = \mathbf{X}\Lambda_k^{-1}$ is the $n \times k$ matrix of the standardized row coordinates called *row standard coordinates*. Equation (5) can be interpreted in terms of *reciprocal averaging* and is called *barycentric property*: the principal coordinate of a category is the average of the standard coordinates of the objects in that category. The corresponding formula is $y_{s\alpha} = \frac{1}{n_s}\sum_{i=1}^{n} g_{is}x^*_{i\alpha} = \bar{x}^*_{s\alpha}$, where $y_{s\alpha}$ is the (s,α)-element of $\mathbf{Y}$ and g_{is} is the (i,s)-element of $\mathbf{G}$ (see Appendix 2 for details on the barycentric property). This barycentric property permits a simultaneous representation of the objects and the categories in the so called *asymmetric map of the columns*.

Contribution and correlation ratio. The absolute contribution of the variable j to the inertia of the column principal component α (αth column of $\mathbf{Y}$) is $c_{j\alpha} = \sum_{s\in\mathcal{M}_j} f_{.s}y^2_{s\alpha}$, where $\mathcal{M}_j$ is the set of categories of variable j. Remembering moreover that $y_{s\alpha} = \bar{x}^*_{s\alpha}$ and the sample mean (resp. variance) of the αth column of $\mathbf{X}^*$ is equal to zero (resp. one), we have the following relation between the absolute contribution $c_{j\alpha}$ and the correlation ratio between the variable j and the row standard component α (αth column of $\mathbf{X}^*$):

$$\eta^2_{j\alpha} = \frac{\sum_{s\in\mathcal{M}_j}\frac{n_s}{n}(\bar{x}^*_{s\alpha} - 0)^2}{1} = p \times c_{j\alpha}. \tag{6}$$

Remembering that in PCA the loadings are correlations between the variables and the components, the correlation ratios, called discrimination measure in Gifi (1990), are interpreted in MCA as *squared loadings*.

The lower rank approximation approach. As shown by Eckart and Young (1936), a rank k least squares approximation of $\widetilde{\mathbf{F}}$ is obtained by selecting in the k largest singular values and corresponding singular vectors. Now, as

$$||\widetilde{\mathbf{F}} - \mathbf{U}_k\Lambda_k\mathbf{V}_k^t||^2 = ||\mathbf{D}_r^{-1}(\mathbf{F} - \mathbf{r}\mathbf{c}^t)\mathbf{D}_c^{-1} - \mathbf{X}^*\mathbf{Y}^t||^2,$$

the matrix $\mathbf{X}^*\mathbf{Y}$ is a rank k least squares approximation of $\mathbf{D}_r^{-1}(\mathbf{F}-\mathbf{r}\mathbf{c}^t)\mathbf{D}_c^{-1}$. This lower rank approximation gives the freedom for rotation in MCA.

3 Simple structure in MCA.

Let $\widetilde{\mathbf{X}}^* = \mathbf{X}^*\mathbf{T}$, and $\widetilde{\mathbf{Y}} = \mathbf{Y}\mathbf{T}$, where $\mathbf{T}\mathbf{T}^t = \mathbf{T}^t\mathbf{T} = \mathbb{I}_k$. Then, as $\mathbf{X}^*\mathbf{Y}^t = \widetilde{\mathbf{X}}^*\widetilde{\mathbf{Y}}^t$, we immediately see that the lower rank approximation is not unique and that the MCA solution $\mathbf{X}^*$ and $\mathbf{Y}$ is not unique over orthogonal rotations. This non-uniqueness can be exploited to improve the interpretability of the original solution by means of rotation. Clearly, rotation of the column principal coordinates matrix $\mathbf{Y}$ to simple structure must be followed by the same rotation of the row standard coordinates matrix $\mathbf{X}^*$. To simplify the interpretation of the correlation ratios, the matrices $\mathbf{Y}$ and $\mathbf{X}^*$ are rotated in such a way that when considering one variable few correlation ratios are large (close to 1) and as many as possible are close to zero.

The Varimax-based function. After rotation of $\mathbf{X}^*$ and $\mathbf{Y}$, the relation (6) remains true:

$$\tilde{\eta}_{j\alpha}^2 = p \sum_{s\in\mathcal{M}_j} f_{.s}\tilde{y}_{s\alpha}^2, \tag{7}$$

where $\tilde{\eta}_{j\alpha}^2$ is the correlation ratio between the variable j and αth column of $\widetilde{\mathbf{X}}^*$. The Kaiser's Varimax function is applied to the $p \times q$ correlation ratio matrix, interpreted as squared correlations, but the rotation matrix $\mathbf{T}$ is applied to $\mathbf{Y}$ which leads to a more complicated function than in PCA:

$$\begin{aligned} h(\mathbf{T}) &= \sum_{\alpha=1}^{k} \left\{ \frac{\sum_{j=1}^{p}(\tilde{\eta}_{j\alpha}^2)^2}{p} - \left(\frac{\sum_{j=1}^{p}\tilde{\eta}_{j\alpha}^2}{p}\right)^2 \right\} \\ &= \sum_{\alpha=1}^{k} \left\{ p\sum_{j=1}^{p}\left(\sum_{s\in\mathcal{M}_j} f_{.s}\tilde{y}_{s\alpha}^2\right)^2 - \left(\sum_{j=1}^{p}\sum_{s\in\mathcal{M}_j} f_{.s}\tilde{y}_{s\alpha}^2\right)^2 \right\}. \end{aligned} \tag{8}$$

The rotation of the $p \times k$ matrix $\mathbf{Y}$ can be formulated as objective,

$$\begin{aligned} \max_{\mathbf{T}} \quad & h(\mathbf{T}), \\ \text{s.t.} \quad & \mathbf{T}\mathbf{T}^t = \mathbf{T}^t\mathbf{T} = \mathbb{I}_k. \end{aligned} \tag{9}$$

The rotation iterative procedure. In PCA, the Kaiser's procedure is aimed at maximizing the sum of variances of the squared columns of $\widetilde{\mathbf{A}}$, where $\widetilde{\mathbf{A}} = \mathbf{AT}$ for a given $p \times k$ matrix $\mathbf{A}$ of factor loadings. Because a direct solution for the optimal $\mathbf{T}$ is not available, except for the case $k = 2$, Kaiser suggested an iterative procedure based on planar rotations. The idea is to alternately rotate all pairs of columns of $\mathbf{A}$. Each rotation is globally optimal for the plane under consideration, and improves the Varimax function, because the contribution of all $k-2$ columns except the pair being rotated is not affected. The essential part of Kaiser's procedure is then the explicit formula of the Varimax angle of rotation.

In MCA, we propose to use the same iterative procedure for the optimization problem (9): the single-plane rotations are made on dimension 1 with 2, 1 with 3, ..., 1 with k, ..., $(k-1)$ with k iteratively until the process converges, i.e. until $\frac{k(k-1)}{2}$ successive rotations providing an angle of rotation equal to zero are obtained. The definition of an explicit formula for the angle of rotation θ maximizing the rotation function h is then the essential part of our proposed generalization of the Kaiser's procedure to MCA.

The planar explicit solution. For $k = 2$, the rotation matrix $\mathbf{T}$ is defined by

$$\mathbf{T} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}. \tag{10}$$

The optimization problem (9) can then be rewritten:

$$\max_{\theta \in \mathbb{R}} h(\theta), \tag{11}$$

where the analytic expression of $h(\theta)$ is given in (19) in Appendix 3. The derivative of h gives (see Appendix 3 for details):

$$\frac{\partial h}{\partial \theta} = 2(a + b\cos(4\theta) + c\sin(4\theta)), \tag{12}$$

where

$$\begin{aligned} a &= (p-1)\sum_{j=1}^{p}\sum_{s\in\mathcal{M}_j}\sum_{t\in\mathcal{M}_j} f_{.s}f_{.t}\alpha_{st}\beta_{st} - \sum_{j=1}^{p}\sum_{l\neq j}\sum_{s\in\mathcal{M}_j}\sum_{t\in\mathcal{M}_l} f_{.s}f_{.t}\alpha_{st}\beta_{st}, \\ b &= (p-1)\sum_{j=1}^{p}\sum_{s\in\mathcal{M}_j}\sum_{t\in\mathcal{M}_j} f_{.s}f_{.t}\delta_{st}\gamma_{st} - \sum_{j=1}^{p}\sum_{l\neq j}\sum_{s\in\mathcal{M}_j}\sum_{t\in\mathcal{M}_l} f_{.s}f_{.t}\delta_{st}\gamma_{st}, \\ c &= \frac{(p-1)}{2}\sum_{j=1}^{p}\sum_{s\in\mathcal{M}_j}\sum_{t\in\mathcal{M}_j} f_{.s}f_{.t}(\gamma_{st}^2 - \delta_{st}^2) - \frac{1}{2}\sum_{j=1}^{p}\sum_{l\neq j}\sum_{s\in\mathcal{M}_j}\sum_{t\in\mathcal{M}_l} f_{.s}f_{.t}(\gamma_{st}^2 - \delta_{st}^2), \end{aligned} \tag{13}$$

with

$$\alpha_{st} = y_{s1}y_{t1} + y_{s2}y_{t2},$$

$$\beta_{st} = y_{s2}y_{t1} - y_{s1}y_{t2},$$

$$\gamma_{st} = y_{s2}y_{t1} + y_{s1}y_{t2},$$

$$\delta_{st} = y_{s1}y_{t1} - y_{s2}y_{t2}. \tag{14}$$

Afterwards the trick to solve $a + b\cos(4\theta) + c\sin(4\theta) = 0$ consists in dividing each term by $(b^2 + c^2)^{1/2}$ and introducing the angle $\varphi \in]-\pi, +\pi]$ such that $\cos(\varphi) = \frac{b}{(b^2+c^2)^{1/2}}$ and $\sin(\varphi) = \frac{c}{(b^2+c^2)^{1/2}}$. It gives

$$\frac{a}{(b^2 + c^2)^{1/2}} + \cos(\varphi)\cos(4\theta) + \sin(\varphi)\sin(4\theta) = \frac{a}{(b^2 + c^2)^{1/2}} + \cos(4\theta - \varphi) = 0.$$

As h only depends on $\cos(\theta)$ and $\sin(\theta)$, it is periodic (of period $\pi/2$) and differentiable and the derivative necessarily cancels for each minimum and maximum. Therefore $|a| \leq (b^2 + c^2)^{1/2}$ and this equation has two solutions:

$$\hat{\theta} = \frac{1}{4}(\pm \arccos(-\frac{a}{(b^2 + c^2)^{1/2}}) + \varphi), \tag{15}$$

corresponding to the minimum and the maximum of h, on condition of course that $|a| \leq (b^2 + c^2)^{1/2}$. But this condition is necessarily verified because as h only depends on $\cos(\theta)$ and $\sin(\theta)$, it is periodic (of period $\pi/2$) and differentiable and the derivative necessarily cancel for each minimum and maximum.

An illustrative example. In this simulated example, we consider four binary variables $x_1, \ldots, x_4$ such that x_1 and x_2 (respectively x_3 and x_4) are strongly linked and not related to the other variables x_3 and x_4 (resp. x_1 and x_2). Then we have two groups of variables denoted $\mathcal{C}_1$ and $\mathcal{C}_2$. Let e_1 (resp. e_2, e_3, e_4) be a category of x_1 (resp. x_2, x_3, x_4) and $\mathbb{P}$ denote one probability measure. To generate a contingency table, the following log-linear model (see for instance Agresti (2002)) is used:

$$\log(\mathbb{P}(x_1 = e_1, \ldots, x_4 = e_4)) = \log(\mu_{e_1e_2e_3e_4})$$
$$= (\lambda^{x_1}_{e_1} + \lambda^{x_2}_{e_2} + \beta^{x_1x_2}_{e_1e_2}) + (\lambda^{x_3}_{e_3} + \lambda^{x_4}_{e_4} + \beta^{x_3x_4}_{e_3e_4}) + \beta^{x_1x_4}_{e_1e_4}, \tag{16}$$

where $e_1, e_2, e_3, e_4 \in \{0, 1\}$. The parameters $\lambda^{x_1}_{e_1}, \lambda^{x_2}_{e_2}, \lambda^{x_3}_{e_3}$ and $\lambda^{x_4}_{e_4}$ designate the effect of each variable and the parameters $\beta^{x_1x_2}_{e_1e_2}$ and $\beta^{x_3x_4}_{e_3e_4}$ are interactions corresponding with cohesion terms in each group. The parameter $\beta_{e_1e_4}^{x_1x_4}$ is used to add some interactions between categories of variables belonging to different groups $\mathcal{C}_1$ and $\mathcal{C}_2$.

We simulate a contingency table corresponding to a global sample size $n = 1000$ using log-linear model (16) with the following values of the parameters $\lambda_0^{x_1} = \lambda_0^{x_3} = 1$, $\lambda_0^{x_2} = \lambda_0^{x_4} = 2$, $\beta_{00}^{x_1x_2} = -1.5$, $\beta_{00}^{x_3x_4} = -0.9$ and $\beta_{00}^{x_1x_4} = -0.5$. All the remaining parameters are set to zero. Thus the within groups cohesion parameters are high whereas the between groups interaction parameters are low in order to get well defined groups. We apply MCA on the categorical data corresponding with the generated contingency table. We retain $k = 2$ components and apply a planar rotation using the Varimax-based function h. Using (15) the corresponding analytic solution is $\hat{\theta} \approx \frac{\pi}{3}$. Figure 1 plots the criterion $h(\theta)$ for $\theta \in [-\pi, \pi]$ and we can verify on this figure that h is $\frac{\pi}{2}$-periodic and maximum in $\hat{\theta} \approx \frac{\pi}{3}$.

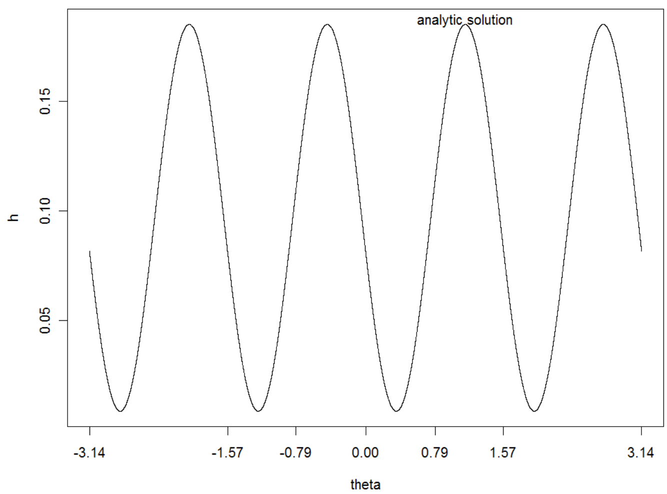

Figure 1: Graph of $\theta \mapsto h(\theta)$.

In order to visualize the impact of rotation on this simulated data, we plot in Figure 2 the four variables according to their correlation ratio to the first row standard component (in abscissa) and to the second row standard component (in ordinate) before and after planar rotation, respectively on the left and right side. As expected the variables are more clearly related to the components after rotation.

Let us also visualize in Figure 3 the impact of rotation on the representation of the categories on the first column principal plane of MCA: the principal coordinates of the categories before (resp. after) rotation are given in the first two columns of $\mathbf{Y}$ (resp. $\widetilde{\mathbf{Y}}$). We see that after rotation the two categories of each

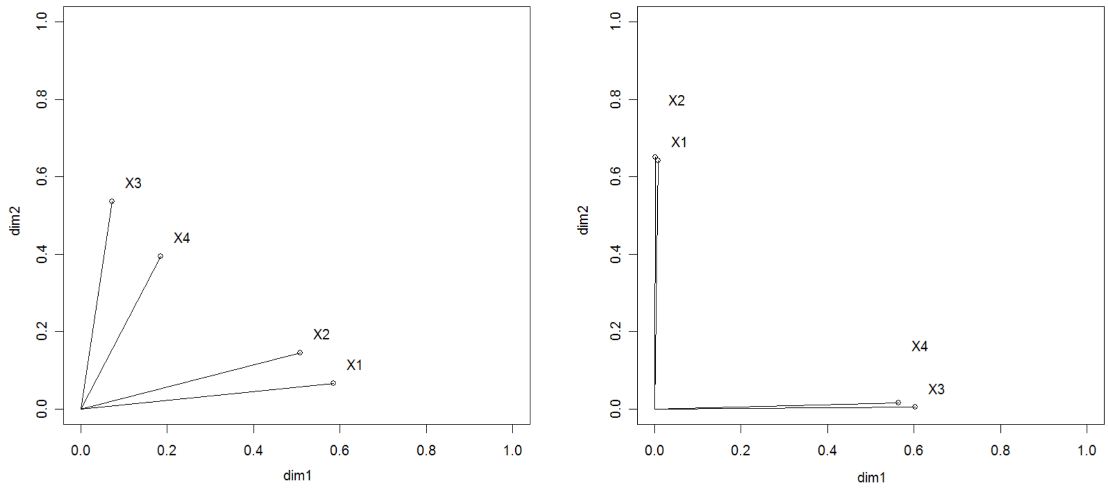

Figure 2: Plot of the correlation ratio matrix before rotation (on the left) and after planar rotation (on the right).

variable are more clearly related to one of the two components. To conclude this simulated example provides expected results. Let us now study the impact of rotation on a real data set.

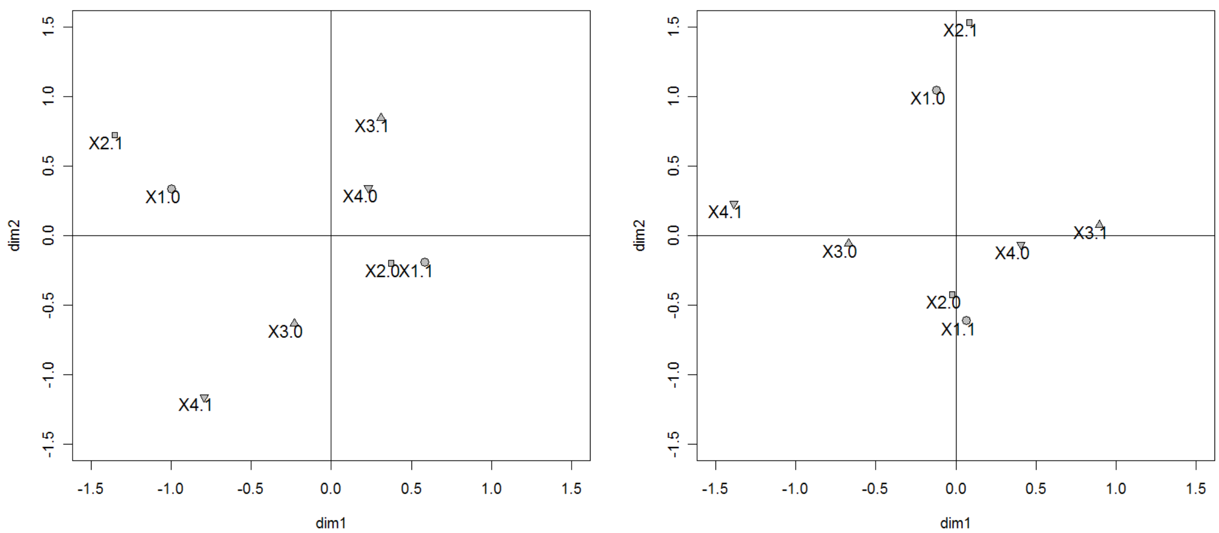

Figure 3: Plot of the categories in the first principal plane before rotation (on the left) and after rotation (on the right).

4 A real data application

In this section we apply this rotation methodology on a real data set in order to illustrate the benefits of using rotation in MCA. We consider a user satisfaction survey of pleasure craft operators on the "Canal des Deux Mers" located in South of France. This study has been realized from June to December 2008. It contains numerous questions with quantitative or qualitative answers. The sample size is $n = 1082$ pleasure craft operators. We focus here on a small number of qualitative variables in order to get clear graphical representations when plotting the categories on the principal plane. Although considering only four variables is of little practical interest, this application is useful to illustrate the rotation phenomenon. The four chosen variables are named "information", "stopover", "cleanliness" and "sailors". They have each one three categories. The variable "information" deals with the quality of the information concerning sites worth visiting and its categories are 1-satisfactory, 2-unsatisfactory and 3-no opinion. The variable "stopover" is associated with the following question *What makes you decide to stop over at a particular place?* and the possible answers are 1-necessity (supplies, time constraints, ...), 2-interest of stopover point (architecture, restaurant, landscape, ...) and 3-desire to be on dry land. The variable "cleanliness" is about the canal's degree of cleanliness (1-clean, 2-average or 3-dirty). Finally the variable "sailors" is associated with the question *How would you describe other sailors you encountered?* and its categories are 1-pleasant, 2-unpleasant and 3-do not know.

To visualize the effects of rotation on this data set, we first plot in Figure 4 the four variables according to their correlation ratio to the first two row standard principal components before and after rotation. We see that the association of the variables to the components is clearly easier after rotation. Thus two groups of variables appear, the first one contains the variables "sailors" and "information" and the second one is composed of "cleanliness" and "stopover".

We observe in Figure 5 the impact of rotation on the representation of the categories on the first principal plane. The rotated components have a better discriminatory capability than the initial ones. The first component represents on the left tourists who decide to stop over at a particular place because of interest and who think the canal's degree of cleanliness is average. On the contrary craft operators on the right stop over because of necessity and find the canal dirty. This component refers to the "expectations of pleasure

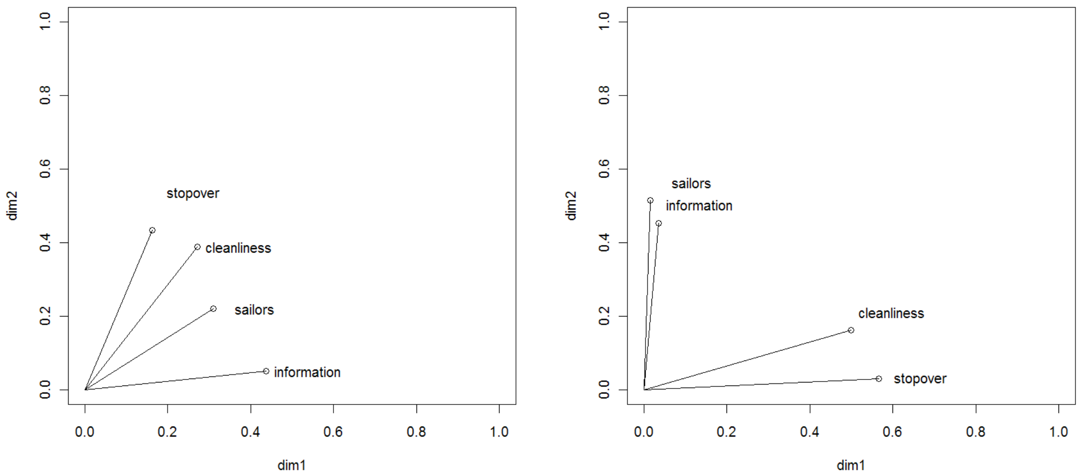

Figure 4: Plot of the correlation ratio matrix before rotation (on the left) and after planar rotation (on the right).

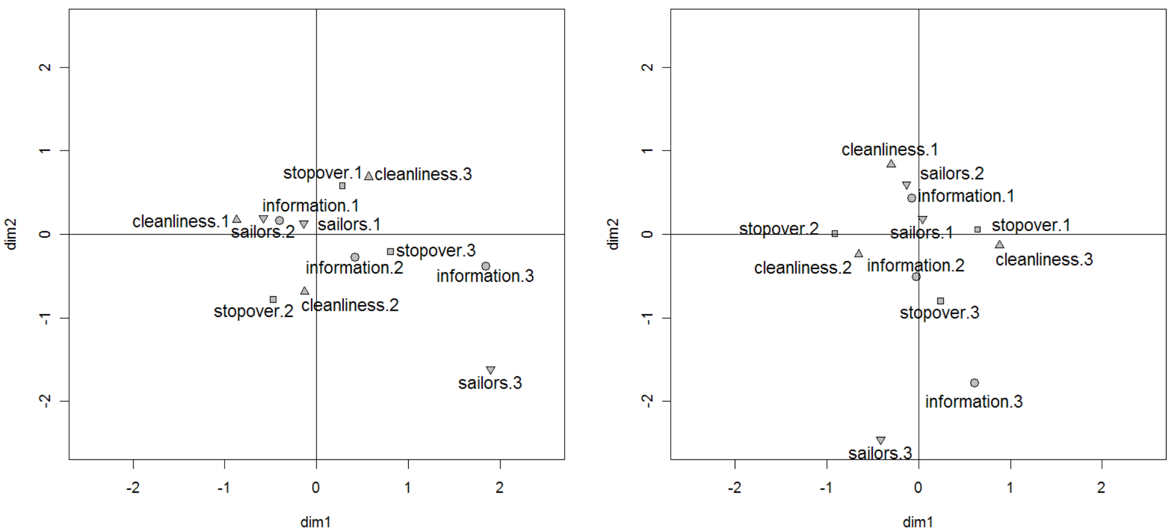

Figure 5: Plot of the categories in the first principal plane before rotation (on the left) and after rotation (on the right).

craft operators" concerning the use of the canal. People who stop over because of necessity may not be pleased to be on dry land and are then quite demanding and critical of the canal out of hand. The second component could be labelled "opinion of the tourists" since it is discriminating between people with and people without an opinion either on the relationship with other sailors or on the information concerning sites worth visiting. Note that a second issue of discussion would be whether the respondents who scored the category 3-do not know when asked their opinion of other sailors are indeed individuals who do not encounter other sailors. Maybe they are people who like some and do not like others. Or people who do not feel like giving their opinion on other sailors. This latter view may be substantiated by the fact that these people also do not give their opinion on the information concerning sites worth visiting. This example on real data shows that rotation in MCA may help for the interpretation of the results since categories are better aligned along the components. Thus the labelling and interpretation of the components is easier.

5 Concluding remarks

In this article we propose a two-dimensional analytic solution for rotation in MCA using a Varimax-based criterion relying on the correlation ratio between the categorical variables and the MCA components. We have checked on a simulated example the accuracy of the given solution. We have also shown that rotation may be beneficial to real data since it may bring new elements for the interpretation of the results. However we are aware of the simplicity of the data we considered for an easier presentation and of the probable supplementary difficulty when dealing with more complex data sets.

When higher dimensionality is required, we use the practical algorithm of Kaiser (1958) which consists in computing the two-dimensional solution and then applying successive pairwise rotations. But although the Kaiser rotation procedure is a very popular techniques in data analysis, it is not without problems. Remedy against nonoptimal Varimax rotation have been proposed (Fraenkel, 1984; ten Berge, 1995) and may possibly be applied in the iterative planar rotation procedures proposed in this paper. ten Berge (1984) also showed that Varimax rotation can be interpreted as a special case of diagonalizing symmetric matrices and that the solution by De Leeuw and Pruzansky (1978) is essentially equivalent to the solution by Kaiser. We would like to obtain the same kind of result in MCA in order to link the rotation procedure proposed by Kiers (1991) for PCAMIX and thus MCA too, and the procedure proposed in this paper.

Moreover we think that the proposed planar solution in MCA can be used in divisive hierarchical methods for the clustering of qualitative variables. The well-known VARCLUS procedure of SAS software, planar rotation is used to help dividing at best a cluster of quantitative variables in two sub-clusters. The adaptation of this approach to qualitative variables is currently under investigation. Finally a future prospect on this work would be to give the analytic expression of the rotation matrix for a dimension larger than two.

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Appendix

Appendix 1: Short recall on row principal coordinates. Let $\mathbf{R} = \mathbf{D}_r^{-1}\mathbf{F} - \mathbf{1}_n\mathbf{c}^t = \mathbf{D}_r^{-1}(\mathbf{F} - \mathbf{r}\mathbf{c}^t)$ denote the $n \times q$ matrix of the centered row profiles. In a first step, MCA (or weighted PCA) searches for an axis with head vector $\mathbf{w}_1$ (of $\mathbf{D}_c^{-1}$-norm equal to 1) such that the vector $\mathbf{x}_1 = \mathbf{R}\mathbf{D}_c^{-1}\mathbf{w}_1$ of the $\mathbf{D}_c^{-1}$-projections of the rows of $\mathbf{R}$, has maximal variance (i.e. a maximal $\mathbf{D}_r$-norm). The first principal component $\mathbf{x}_1$ is then solution of the optimization problem:

$$\begin{cases} \max\limits_{\mathbf{x} \in \mathbb{R}^n} \parallel \mathbf{x} \parallel^2_{\mathbf{D}_r}, \\ \text{subject to } \mathbf{w}^t\mathbf{D}_c^{-1}\mathbf{w} = 1, \end{cases} \tag{17}$$

which is equivalent, with the change of variable $\mathbf{v} = \mathbf{D}_c^{-1/2}\mathbf{w}$, to the following simpler writting:

$$\begin{cases} \max\limits_{\mathbf{v} \in \mathbb{R}^p} \mathbf{v}^t\widetilde{\mathbf{F}}^t\widetilde{\mathbf{F}}\mathbf{v}, \\ \text{s.t.} \mathbf{v}^t\mathbf{v} = 1. \end{cases} \tag{18}$$

where $\widetilde{\mathbf{F}} = \mathbf{D}_r^{-1/2}(\mathbf{F} - \mathbf{r}\mathbf{c}^t)\mathbf{D}_c^{-1/2}$. The first eigenvector $\mathbf{v}_1$ associated with the largest eigenvalue λ_1 of the matrix $\widetilde{\mathbf{F}}^t\widetilde{\mathbf{F}}$ is a solution of (18) and the sample variance of $\mathbf{x}_1$ is equal to λ_1. The other principal components are defined similarly by $\mathbf{x}_\alpha = \mathbf{R}\mathbf{D}_c^{-1/2}\mathbf{v}_\alpha$, for $\alpha = 2, \dots k$, where $\mathbf{v}_\alpha$ is the eigenvector associated with the αth largest eigenvalue λ_α of $\widetilde{\mathbf{F}}^t\widetilde{\mathbf{F}}$ and λ_α is the sample variance of $\mathbf{v}_\alpha$. The vectors $\mathbf{x}_\alpha$ are the k columns of the matrix of object scores $\mathbf{X} = \mathbf{R}\mathbf{D}_c^{-1/2}\mathbf{V}_k = \mathbf{D}_r^{-1/2}\widetilde{\mathbf{F}}\mathbf{V}_k$.

Appendix 2: The barycentric property. Equation (4) of the column principal coordinate matrix gives $\mathbf{Y}^t = \Lambda_k\mathbf{V}_k^t\mathbf{D}_c^{-1/2}$. It follows from (3), that $\widetilde{\mathbf{F}}\mathbf{D}_c^{-1/2} = \mathbf{U}_k\mathbf{Y}^t$ and from (4) that $\mathbf{Y} = \mathbf{D}_c^{-1}(\mathbf{F} - \mathbf{r}\mathbf{c}^t)^t\mathbf{D}_r^{-1/2}\mathbf{U}_k = \mathbf{D}_c^{-1}(\mathbf{F} - \mathbf{r}\mathbf{c}^t)^t\mathbf{X}^*$.

Remembering from the definition of $\mathbf{F}$ that $f_{is} = \frac{g_{is}}{np}$, $f_{i.} = \frac{1}{n}$ and $f_{.s} = \frac{n_s}{np}$, the general term of $(\mathbf{F} - \mathbf{r}\mathbf{c}^t)$

is then $\frac{g_{is}}{np} - \frac{n_s}{n^2p}$. It gives:

$$\begin{aligned} y_{s\alpha} &= \sum_{i=1}^{n} \frac{np}{n_s}(\frac{g_{is}}{np} - \frac{n_s}{n^2p})x^*_{i\alpha} \\ &= \frac{1}{n_s}\sum_{i=1}^{n} g_{is}x^*_{i\alpha} - \frac{1}{n}\sum_{i=1}^{n} x^*_{i\alpha} \\ &= \bar{x}^*_{s\alpha} \end{aligned}$$

Appendix 3: Analytic expression of $h(\theta)$. For $k=2$, criterion (8) simply writes

$$h(\theta) = \underbrace{p\sum_{j=1}^{p}\left(\sum_{s\in\mathcal{M}_j} f_{.s}\tilde{y}_{s1}^2\right)^2}_{M_1} + \underbrace{p\sum_{j=1}^{p}\left(\sum_{s\in\mathcal{M}_j} f_{.s}\tilde{y}_{s2}^2\right)^2}_{M_2} - \underbrace{\left(\sum_{j=1}^{p}\sum_{s\in\mathcal{M}_j} f_{.s}\tilde{y}_{s1}^2\right)^2}_{M_3} - \underbrace{\left(\sum_{j=1}^{p}\sum_{s\in\mathcal{M}_j} f_{.s}\tilde{y}_{s2}^2\right)^2}_{M_4} \quad (19)$$

where $\tilde{y}_{s1} = y_{s1}\ \cos\theta + y_{s2}\ \sin\theta$ and $\tilde{y}_{s2} = -y_{s1}\ \sin\theta + y_{s2}\ \cos\theta$ are the rotated loadings.

To maximize (19), we have to differentiate h with respect to θ and to set the derivative equal to zero. Note that this is only a necessary but not sufficient condition and we have to make sure it is a maximum. Let us first remark that $\dfrac{\partial\tilde{y}_{s1}}{\partial\theta} = \tilde{y}_{s2}$ and $\dfrac{\partial\tilde{y}_{s2}}{\partial\theta} = -\tilde{y}_{s1}$. Thus we have

$$\frac{\partial(M_1+M_2)}{\partial\theta} = 4pA \quad \text{and} \quad \frac{\partial(M_3+M_4)}{\partial\theta} = 4(A+B)$$

where

$$A = \sum_{j=1}^{p}\left\{(\sum_{s\in\mathcal{M}_j} f_{.s}\tilde{y}_{s1}\tilde{y}_{s2})(\sum_{t\in\mathcal{M}_j}(\tilde{y}_{t1}^2 - \tilde{y}_{t2}^2))\right\}$$

and

$$B = \sum_{j=1}^{p}\sum_{l\neq j}^{p}(\sum_{s\in\mathcal{M}_j} f_{.s}\tilde{y}_{s1}\tilde{y}_{s2})(\sum_{t\in\mathcal{M}_l} f_{.t}(\tilde{y}_{t1}^2 - \tilde{y}_{t2}^2)).$$

It follows $\dfrac{\partial h}{\partial\theta} = 4(p-1)A - 4B$. Let us now remark that $\tilde{y}_{s1}\tilde{y}_{s2} = (y_{s2}^2 - y_{s1}^2)\frac{1}{2}\sin2\theta + y_{s1}y_{s2}\cos2\theta$, and $\tilde{y}_{t1}^2 - \tilde{y}_{t2}^2 = (y_{t1}^2 - y_{t2}^2)\cos2\theta + 2y_{t1}y_{t2}\sin2\theta$. Then we have

$$A = \sum_{j=1}^{p}\left\{\{\sum_{s\in\mathcal{M}_j} f_{.s}[(y_{s2}^2 - y_{s1}^2)\frac{1}{2}\sin2\theta + y_{s1}y_{s2}\cos2\theta]\} \times \{\sum_{t\in\mathcal{M}_j} f_{.t}[(y_{t1}^2 - y_{t2}^2)\cos2\theta + 2y_{t1}y_{t2}\sin2\theta]\}\right\}.$$

After a good deal of trigonometric identities and algebraic manipulations, we get:

$$\begin{aligned} A = \tfrac{1}{2}\textstyle\sum_{j=1}^{p}\sum_{s\in\mathcal{M}_j}\sum_{t\in\mathcal{M}_j} f_{.s}f_{.t} \quad &\{(y_{s2}^2 - y_{s1}^2)y_{t1}y_{t2} + (y_{t1}^2 - y_{t2}^2)y_{s1}y_{s2} \\ &+[(y_{s1}^2 - y_{s2}^2)y_{t1}y_{t2} + (y_{t1}^2 - y_{t2}^2)y_{s1}y_{s2}] \times \cos4\theta \\ &+\tfrac{1}{2}[(y_{s2}^2 - y_{s1}^2)(y_{t1}^2 - y_{t2}^2) + 2y_{s1}y_{s2}y_{t1}y_{t2}] \times \sin4\theta\}. \end{aligned}$$

Then we have

$$A = \frac{1}{2}\sum_{j=1}^{p}\sum_{s\in\mathcal{M}_j}\sum_{t\in\mathcal{M}_j} f_{.s}f_{.t}\{\alpha_{st}\beta_{st} + \delta_{st}\gamma_{st}\cos4\theta + \frac{1}{2}(\gamma_{st}^2 - \delta_{st}^2)\sin4\theta\}$$

and

$$B = \frac{1}{2}\sum_{j=1}^{p}\sum_{l\neq j}^{p}\sum_{s\in\mathcal{M}_j}\sum_{t\in\mathcal{M}_j} f_{.s}f_{.t}\{\alpha_{st}\beta_{st} + \delta_{st}\gamma_{st}\text{cos}4\theta + \frac{1}{2}(\gamma_{st}^2 - \delta_{st}^2)\text{sin}4\theta\}$$

where the terms α_{st}, β_{st}, γ_{st} and γ_{st} are defined in (14). Finally, we get:

$$\frac{\partial h}{\partial \theta} = 2(a + b\text{cos}4\theta + c\text{sin}4\theta),$$

where the expression of a, b and c are given in (13).

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