Three-way compositional data analysis

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For the exploratory analysis of three-way data, e.g., measurements of a number of objects, on a number of variables at different points in time, Tucker analysis is one of the most applied technique to study three-way array when the data are approximately trilinear. It can be considered a three way generalization of PCA (Principal Component Analysis). Like PCA, to interpret the results from these methods, it is possible, in addition to inspecting the loadings matrices and core array, inspect visual representation of the outcome. When the data are particular ratios, as in the case of compositional data, these models should consider the special problems that compositional data gives. Aim of this work is describe how an analysis of compositional data by Tucker analysis is possible and how the results should be interpreted. Moreover, a procedure for displaying the results for objects, variables and occasions will be given.

Keywords: Tucker analysis, logratio trasformation, vector of juxtaposed compositions, one mode plot, relative variation parts plot.

1. Introduction

Compositional data, consisting of such vectors of proportions, are generally arranged into a matrix, when each composition is one row. Sometimes, compositional data are arranged into three-way array, e.g. proportions of different chemical compounds in several rivers at the different seasons. In these cases, one of the typical purposes of using three-way analysis is exploring the interrelations in data. PARAFAC/CANDECOM (Harsman, 1970; Caroll and Chang, 1970 - PC) and Tucker models (Tucker, 1966; Kroonenberg and de Leeuw, 1980) are the methods particularly suitable for the exploratory analysis. Both yield a low-dimensional descriptions of the three-way compositional data and, like PCA on two-way matrix of compositional data, their have proved difficult to handle statistically because of the awkward constraint that the components of each vector must sum to unity. Gallo et *al*. (2008) has proposed a reexamination of PC and Tucker3 model based on a certain choice of prerequisites which the PC of compositional data should reasonably be expected to satisfy, i.e., scale invariante and subcompositional coherence.

The principal purpose of this paper is explain a plotting procedure for visualizing the Tucker results of compositional data without pitfalls of interpretation. Thus, in Paragraph 2 we recall briefly the principal characteristics of compositional data. In Paragraph 3, once examined the pretreatment of compositional data, the properties and the relative geometry is considerate for the compositional data arranged into flatted matrices. In Paragraph 4 Tucker models for compositional data are given. The procedure for plotting each single mode is shown in Paragraph 5. Finally, an application of Tucker2 model is given in Paragraph 6.

2. Compositional data

A row vector of compositional data, $\mathbf{v}_i = (v_{i1},\ldots,v_{iJ})$, can be defined as *J*-part composition where all its components are strictly positive quantities and its sum is always a constant κ . Several units are possible define, where the most common examples are $\kappa = 1$, which means that measurements have been made in part per unit, and $\kappa = 100$, for measurements in percent. In mathematical term, any vector $\tilde{\mathbf{v}}_i = (\tilde{v}_{i1},\ldots,\tilde{v}_{iJ})$ with $\tilde{v}_{i1} > 0,\ldots,\tilde{v}_{iJ} > 0$ can be transformed into a compositional vector

$\mathbf{v}_i$ by a closure operator $\mathbb{C}$. The closure of $\tilde{\mathbf{v}}_i$ is defined as $\mathbb{C}(\tilde{\mathbf{v}}_i) = \left(\kappa\tilde{v}_{i1}/\|\tilde{\mathbf{v}}_i\|,\ldots,\kappa\tilde{v}_{iJ}/\|\tilde{\mathbf{v}}_i\|\right)$, where $\|.\|$ is the trace of vector. The closure operator defines a transformation $\Re_+^J \to S^J$ where $\Re_+^J$ is the positive orthant of $\Re^J$ and the simplex S^J is the sample space of compositional data, defined as $S^J = \left\{(v_{i1},\ldots,v_{iJ}):\ v_{i1}>0,\ldots,v_{iJ}>0;\ \sum_{j=1}^{J} v_{ij} = \kappa\right\}$.

Thus, when κ changes, the sum of compositional vector changes but the analysis should yield the same results, independently of the value of κ. The principal conditions should be fulfilled by any statistical method to be applied to composition data are scale invariance and subcompositional coherence. These conditions should have been sufficient to warn against the study of compositional data analysis by 'standard' multiway methodology. In fact, according to principle of scale invariance, compositional data analysis provides information only about relative values. Moreover, in according to principle of subcompositional coherence, when the distance between two full compositions is measured it must be greater, or at least equal, then the distance between them when considering any subcomposition. For full details on structure of the simplex and relative geometry see Aitchison (1986) and Pawlowsky-Glahn et *al.* (2007).

3. Pretreatment of compositional data into three-way array

When compositional vectors are observed in several occasions they can be arranged in a three-way array as rows, columns or tubes. In this paper, the three-way array $\underline{\mathbf{V}}$ $(I \text{ x } J \text{ x } K)$ has $(I \text{ x } K)$ rows, where each row $\mathbf{v}_i^k$ $(i=1,...,I;\ k=1,...,K)$ is a composition vector, the J columns corresponding to the parts or components of composition. While $\underline{\mathbf{v}}_i = \left[\mathbf{v}_i^1|\ldots|\mathbf{v}_i^k|\ldots|\mathbf{v}_i^k\right]$ is a JK-dimensional vector where ith object is observed into K different simplex spaces, ones for each occasion: $\mathbf{v}_i^k \in S_k^J$ $(k=1,...,K)$. In other words, $\mathbf{v}_i^k$ is a compositional J-dimensional vector observed in kth occasion, and $\underline{\mathbf{v}}_i$ is a vector of juxtaposed compositions. Finally, we define $\mathbf{V}_k$ $(I \text{ x } J)$ a matrix obtained by fixing the third mode of $\underline{\mathbf{V}}$ at k ($\mathbf{V}_k$ is the kth frontal slice of $\underline{\mathbf{V}}$).

Into context of exploratory analysis, a lot of research was devoted to finding a useful transformation of compositional data from simplex to the usual real space. Once the multivariate methods are applied to the transformed data, the results are back-transformed to the original simplex space.

This strategy results was than for each element of row $\mathbf{v}_i^k$ the logarithms of the ratios $v_{ijk}/v_{ij'k}$, known as logratio, between all pairs of parts $(j<j')$ are considered (Aitchison, 1982). Thus, for each vector $\mathbf{v}_i^k$ a new vector with $(J-1)J/2$ logratios is given. These vector are arranged how rows in three-way array $\underline{\hat{\mathbf{Z}}}$ $\left(I \text{ x } J(J-1)/2 \text{ x } K\right)$ where the typical element is $\log\left(v_{ijk}/v_{ij'k}\right)$. Through this transformation, a direct association between the Euclidean metric structure and the simplex space is searched, where it is well known the linear vector space structure for the composition vector $\mathbf{v}_i^k$, for more detail see Pawlowsky-Glahn et *al.*, 2007. These results can be generalized for the vector $\underline{\mathbf{v}}_i$, see appendix A for full details.

Others logratios transformation proposed in literature are additive logratio (*alr*), no discuss it, centred logratio transformation (*clr*), and the isometric logratio (*ilr*) transformation. The *alr* and *clr* were introduced by Aitchison (1982), while *ilr* was introduced by Egozcue et *al.* (2003).

The *clr* transformation of v_{ijk} is the logarithmic transformation of ratios between the elements of compositional vector v_{ijk} and the geometric mean of $\mathbf{v}_i^k$: $z_{ijk} = \log\left(v_{ijk} / g\left(\mathbf{v}_i^k\right)\right)$ with $g\left(\mathbf{v}_i^k\right) = g(v_{i1k} v_{i2k} \cdots v_{iJk})^{1/J}$. Thus, the three-way array $\underline{\mathbf{Z}}$ $(I \text{ x } J \text{ x } K)$, with typical element z_{ijk} and typical row $\mathbf{z}_i^k = \left[z_{i1k},\ldots,z_{iJk}\right] = clr\left(\mathbf{v}_i^k\right) = \left[\log\left(v_{i1k} / g\left(\mathbf{v}_i^k\right)\right),...,\log\left(v_{iJk} / g\left(\mathbf{v}_i^k\right)\right)\right]$, is smaller of pairwise logratios array $\underline{\widehat{\mathbf{Z}}}$. The isometric logratio (*ilr*) transformation of $\mathbf{v}_i^k$ is given by $\breve{\mathbf{z}}_i^k = \left[\breve{z}_{i1k},\ldots,\breve{z}_{iJk}\right] = \left[\log\left(v_{i1k}\right),\ldots,\log\left(v_{iJk}\right)\right]\Psi$ with $\Psi\Psi^t = \mathbf{I}_{J-1}$ and $\Psi^t\Psi = \left(\mathbf{I}_J - \hat{\mathbf{1}}_J\hat{\mathbf{1}}_J^t / J\right)$, $\mathbf{I}_J$ is $\left(J \text{ x } J\right)$ identity matrix and $\hat{\mathbf{1}}_J$ is a vector of units of *J* dimension.

Fortunately all these transformations are strictly linked, in fact, it will show than all the Tucker results about $\underline{\widehat{\mathbf{Z}}}$ can be given by the analysis of the smaller array $\underline{\mathbf{Z}}$. Moreover, it is easy verify than $\breve{\mathbf{z}}_i^k = {}^+\mathbf{z}_i^k = clr\left(\mathbf{v}_i^k\right)\Psi$, thus the centred logratio can be expressed how coordinate into orthonormal space too. Thus, following the works on two-way matrix (Aitchison, 1986; Egozcue et *al.*, 2003), it is known than the distance between two compositional vector, e.g. $d_a\left(\mathbf{v}_i^k, \mathbf{v}_{i'}^k\right)$, into simplex S_k^J , known as Aitchison distance, is equivalent to the ordinary Euclidean distance in $\Re^{J-1}$, e.g. $d\left({}^+\mathbf{z}_i^k, {}^+\mathbf{z}_{i'}^k\right)$. And it follows than $d_\alpha^2\left(\underline{\mathbf{v}}_i, \underline{\mathbf{v}}_{i'}\right) = \sum_{k=1}^K d_\alpha^2\left(\mathbf{v}_i^k, \mathbf{v}_{i'}^k\right) = d^2\left({}^+\underline{\mathbf{z}}_i, {}^+\underline{\mathbf{z}}_{i'}\right)$ where ${}^+\underline{\mathbf{z}}_i = \left[{}^+\mathbf{z}_i^1 \middle| .. \middle| {}^+\mathbf{z}_i^k \middle| ... \middle| {}^+\mathbf{z}_i^K\right]$. In other words, results that could be obtained using a vector of the juxtaposed compositions $\underline{\mathbf{v}}_i$ are exactly the same as those obtained using the coordinates of the juxtaposed compositions ${}^+\underline{\mathbf{z}}_i$ and using the ordinary Euclidean geometry.

Unfortunately, the logratio transformations remove the effect due to mean for the compositions, but the parts of composition preserve their means, where they are rarely of importance in exploratory analysis. Thus, single centering performed successively across two way are referred to as double centering (Smilde et *al.*, 2004), i.e., double centering is performed by first centering across first way and then centering the outcome across the second ones. Let $\mathbf{Z}_k$ be *k*th frontal slice of $\underline{\mathbf{Z}}$, then center $\mathbf{Z}_k$ respect to column means is possible by the symmetric and idempotent centering matrix $\mathbf{P}_I^\perp = \left(\mathbf{I}_I - \hat{\mathbf{1}}_I\hat{\mathbf{1}}_I^t / I\right)$ where $\mathbf{I}_I$ is $\left(I \text{ x } I\right)$ identity matrix and $\hat{\mathbf{1}}_I$ is a vector of units of *I* dimension: $\mathbf{Y}_k = \mathbf{P}_I^\perp\mathbf{Z}_k$. In this way, each frontal slice of $\underline{\mathbf{Y}}$ is double-centered: $\mathbf{Y}_k\hat{\mathbf{1}}_J = \hat{\mathbf{0}}_I$ and $\hat{\mathbf{1}}_I\mathbf{Y}_k = \hat{\mathbf{0}}_J$ where $\hat{\mathbf{0}}_J$ is a vector of zero of *J* dimension.

When centering is performed on the $\mathbf{Z}_k$ columns the system of coordinates of any composition is shifted to the barycentre of the simplex S_k^J while the geometry is conserved (Pawlowsky-Glahn et *al.*, 2007).

4. Three-way Tuker analysis

Tucker analysis, known as N-mode principal component analysis, is a three-way generalization of principal component analysis where loadings matrices are employed for each mode. A different number of loadings can be used in the different modes and the relations between the loadings of each modes are captured by a three-way array $\underline{\mathbf{G}}$ called 'core' array. Specifically, let $\underline{\mathbf{G}}$

$(P \text{ x } Q \text{ x } R)$ and $\underline{\mathbf{E}}$ $(I \text{ x } J \text{ x } K)$ be the core- and the residual- array respectively, in Kronecker product notation, Tucker3 model can be written

$$\mathbf{Y}_A = \mathbf{A}\mathbf{G}_A\left(\mathbf{C}^t \otimes \mathbf{B}^t\right) + \mathbf{E}_A \qquad (1)$$

where $\mathbf{Y}_A$ $(I \text{ x } JK)$ is given by juxtaposition of $\left[\mathbf{Y}_1|\ldots|\mathbf{Y}_k|\ldots|\mathbf{Y}_K\right]$, $\mathbf{A}$ $(I \text{ x } P)$, $\mathbf{B}$ $(J \text{ x } Q)$ and $\mathbf{C}$ $(K \text{ x } R)$ are the loadings matrices for first-, second- and third- mode, where for the double-centred on each matrix $\mathbf{Y}_k$ the loadings matrices for the first two modes must have column sum equal to zero: $\hat{\mathbf{1}}_I\mathbf{A} = \hat{\mathbf{0}}_P$ and $\hat{\mathbf{1}}_J\mathbf{B} = \hat{\mathbf{0}}_Q$. Let $\mathbf{G}_A = \left[\mathbf{G}_1|\ldots|\mathbf{G}_r|\ldots|\mathbf{G}_R\right]$ be the matricized of core-array, where $\mathbf{G}_r$ is rth frontal slice of size $(P \text{ x } \mathrm{Q})$ and the generic element gives the interaction between factors, $\mathbf{E}_A = \left[\mathbf{E}_1|\ldots|\mathbf{E}_k|\ldots|\mathbf{E}_K\right]$ is the matricized of residual array with dimension $(I \text{ x } JK)$.

In Tucker3 all three modes are reduced with P, Q, R the number of factors for first-, second- and third- mode ($P < I$, $Q < J$ and $R < K$). Differently, in Tucker2 only two of three modes are reduced, i.e. first and second mode, in this case the model can be written

$$\mathbf{Y}_C = \mathbf{G}_C\left(\mathbf{A}^t \otimes \mathbf{B}^t\right) + \mathbf{E}_C \quad (2)$$

with $\mathbf{Y}_C$ $(K \text{ x } JI)$ the juxtaposition of $\left[\mathbf{Y}_1^t|\ldots|\mathbf{Y}_j^t|\ldots|\mathbf{Y}_J^t\right]$, $\mathbf{G}_C = \left[\mathbf{G}_1^t|\ldots|\mathbf{G}_q^t|\ldots|\mathbf{G}_Q^t\right]$ the matricized of core-array, with $\mathbf{G}_q^t$ is qth vertical slice of size $(R \text{ x } P)$, and $\mathbf{E}_C = \left[\mathbf{E}_1^t|\ldots|\mathbf{E}_j^t|\ldots|\mathbf{E}_J^t\right]$ is the matricized of residual array with $\mathbf{E}_j^t$ is jth vertical slice of size $(K \text{ x } I)$.

Finally, with Tucker1 only one of three modes is reduce, e.g. first mode, in this case the model can be written

$$\mathbf{Y}_A = \mathbf{A}\mathbf{G}_A + \mathbf{E}_A \quad (3)$$

Exist a hierarchical relationship between these models, moreover the principal component analysis (PCA) as a special case of Tucker model. In fact, a general Tucker framework can be seen as attempts to model as a multiplication of score and loading matrices (Smilde et *al.*, 2004, pp.75). In formal term,

$$\mathbf{Y}_A = \mathbf{A}\mathbf{W}_A^t + \mathbf{E}_A \quad (4)$$

where $\mathbf{A}$, $\mathbf{Y}_A$ and $\mathbf{E}_A$ are defined before, and the loading matrix $\mathbf{W}_A$ $(I \text{ x } JK)$ represent the different three-way structure. Thus, we have $\mathbf{W}_A = (\mathbf{C} \otimes \mathbf{B})\mathbf{G}_A^t$, in case of Tucker3, $\mathbf{W}_A = (\mathbf{I} \otimes \mathbf{B})\mathbf{G}_A^t$, in case of Tucker2, $\mathbf{W}_A = \mathbf{G}_A^t$, in case of Tucker1, and $\mathbf{W}_A = \mathbf{B}$ in case of PCA.

In order to estimating the parameters of the models, several algorithms are proposed in literature. Considering the bilinear model (4) a direct closed-form to the problem is the singular value decomposition (SVD) of $\mathbf{Y}_A$ than, in case of PCA and Tucker1, provide a direct fit of all

parameters. In case of Tucker3 and Tucker2 model, solving the equation (4) provide a direct fit of $\mathbf{A}$ while the others parameters are confused into $\mathbf{W}_A$. This problem can be solved in two steps. First, as to determine the loadings $\mathbf{A}$ is to take the first *P* left singular vectors of $\mathbf{Y}_A$. Similarly, the loadings $\mathbf{B}$ and $\mathbf{C}$ can be given by the first Q and R left singular vectors of $\mathbf{Y}_B$ and $\mathbf{Y}_C$, respectively. And once fitted $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ (for Tucker2 $\mathbf{C}=\mathbf{I}_K$), the core-array can subsequently be calculated as $\mathbf{G}_A=\mathbf{A}^t\mathbf{Y}_A\left(\mathbf{C}\otimes\mathbf{B}\right)$ (for full details see Smilde et *al.*, 2004, pp.120). Thus, the loadings are the singular values decomposition of $\underline{\mathbf{Y}}$ matricized on different ways, and core-array contains the strength (or weight) of the linkage between the loadings of the different modes.

5. Graphical displays

In additional to inspecting the loadings matrices, several displaying procedures can be used to facilitate the interpretation of Tucker results. Kroonenberg (2008) and Kiers (2000) discussed several types of plots: one mode plot in which the elements of a single mode are plotted such components against the elements of the two others combined modes, joint biplot in which the elements of one mode to the elements of one other mode are displayed for each of the elements in the third mode, nested-mode plot in which are plotted such combined elements against each other to obtain trajectories. Of course, in case of compositional data to respect the nature of data and the preprocessing on them, the graphical display procedure must assure orthonormal basis and more attention should be payed when the plots are inspected.

Here a graphical display for each dimension separately, against the elements of the two others combined modes is proposed, where the role assigned to the three modes are different. Thus, *I* objects should be plotted into *P*-dimensional orthonormal space and, at the same time, their loadings should be have zero-sum (due to double-centred preprocessing on the data). In mathematical term, we are looking for a matrix $\mathbf{W}_A$ such that $\mathbf{W}_A^t\mathbf{W}_A=\mathbf{I}_P$ and a loadings matrix $\mathbf{A}$ such that $\hat{\mathbf{1}}_I\mathbf{A}=\hat{\mathbf{0}}_P$ where $\hat{\mathbf{0}}_P$ is a vector of zero. Similarly, for the plot of *J* parts we have to find a Q-dimension orthonormal space $\left(\mathbf{W}_B^t\mathbf{W}_B=\mathbf{I}_Q\right)$ and loadings with zero-sum $\hat{\mathbf{1}}_J\mathbf{B}=\hat{\mathbf{0}}_Q$. Regarding the *K* occasions, there are plotted into an *R*-dimensional orthonormal space, however, due to pretreatment on original data, they have not a particular interpretation therefore it is not considered here (for its interpretation see Kroonenberg, 2008 or Smilde et *al.*, 2004).

5.1 Plotting objects

Let $\underline{\mathbf{v}}_i$ and $\underline{\mathbf{v}}_{i'}$ be two *JK*-dimensional vectors with *i*th and *i'*th objects observed into *K* different simplex spaces, their coefficients for $\Re^{JK}$ is arranged into *i*th and *i'*th row of $\mathbf{Y}_A$. We have seen than the distance between the two vectors into *K* simplex spaces is equivalent their ordinary Euclidean distance. Now, Tucker analysis searches for the *I* objects a low-dimensional subspace, where the $I(I-1)/2$ pairwise distances between the objects should be preserved as well as possible given the reduced dimensionality of space.

In Section 4 we have seen than the loadings for objects are given by the SVD of flatted array of centred logratio transformation of compositional data, $\mathbf{Y}_A$, where we are interested to evaluate the pairwise logratios. Generalizing the results of Aitchison and Greenacre (2002), in Appendix B is showed than studying the centred logratios data it is possible to obtain all the results about the pairwise logratios data where the only difference is that the singular values differ by the constant

factor $\sqrt{J}$. Finally, to preserve the Euclidean distance between the *I* objects observed in *K* occasions, we have to find an orthonormal basis for $\mathbf{A}$. Now, due two double-centred of each $\mathbf{Y}_k$ $(k = 1,\ldots,K)$, the SVD of $\mathbf{Y}_A$ assure than the matrix of left singular vectors $\mathbf{A}$ is orthonormal and column centred, nevertheless the basis $\mathbf{W}_A$ is just orthogonal and not orthonormal: $\mathbf{W}_A^t\mathbf{W}_A = \mathbf{G}_A\left(\mathbf{C}^t \otimes \mathbf{B}^t\right)\left(\mathbf{C} \otimes \mathbf{B}\right)\mathbf{G}_A^t = \mathbf{G}_A\mathbf{I}_{QR}\mathbf{G}_A^t$. In this form, $\mathbf{A}$ is an orthonormal score matrix, therefore, if it is plotted the Euclidean distance between their elements are not preserved. For the purpose to plot the objects into orthonormal subspace, following Kiers (2000), we propose to find a transformation $\mathbf{T}_A$ matrix such that $\hat{\mathbf{W}}_A = \mathbf{W}_A\mathbf{T}_A$ is columnwise orthonormal (i.e. Gram-Schmidt orthonormalization), and postmultiply $\mathbf{A}$ by $\left(\mathbf{T}_A^t\right)^{-1}$ we have $\mathbf{Y}_A = \mathbf{A}\mathbf{W}_A^t = \hat{\mathbf{A}}\hat{\mathbf{W}}_A^t$ with $\hat{\mathbf{A}} = \mathbf{A}\left(\mathbf{T}_A^t\right)^{-1}$.

In this form, $\hat{\mathbf{A}}$ can be referred to coordinates, as principal coordinates, into an *P*-orthonormal subspace of $\Re^{JK}$. In fact, the sum of square of the coordinate of points along the axes is the sum of squares of core-matrix elements, then dividing the sum of square of the coordinate of points along each axis by the total sum of squares, we get the proportion of the variability explained (Kroonenberg, 2008 pp.226). Moreover, the matrix $\hat{\mathbf{A}}$ has column sum equal to zero, then the centre of plot coincides with the centre of gravity of the objects. The distances between the *I* points are the approximation of the distances between the *I* objects observed in *K* different occasions. However, the estimated distance between each couple of objects are always less than the exact value observed through the *K* simplex spaces.

5.2 Plotting parts

Based on the symmetric property of Tucker models to obtain a one mode plot for the *J* parts, we can applied the same procedure used for plotting the *I* objects. Let $\mathbf{Y}_B$ be given by juxtaposition of $\left[\mathbf{Y}_1^t|\ldots|\mathbf{Y}_k^t|\ldots|\mathbf{Y}_K^t\right]$, the SVD of $\mathbf{Y}_B$ assure than the matrix of left singular vectors $\mathbf{B}$ is orthonormal and column centred, and the basis is orthogonal: $\mathbf{W}_B^t\mathbf{W}_B = \mathbf{G}_B\left(\mathbf{C}^t \otimes \mathbf{A}^t\right)\left(\mathbf{C} \otimes \mathbf{A}\right)\mathbf{G}_B^t = \mathbf{G}_B\mathbf{I}_{PR}\mathbf{G}_B^t$, where $\mathbf{G}_B = \left[\mathbf{G}_1^t|\ldots|\mathbf{G}_r^t|\ldots|\mathbf{G}_R^t\right]$ is the matricized of core-array, $\mathbf{G}_r$ is *r*th frontal slice of size $(P \text{ x } Q)$, and $\mathbf{I}_{PR}$ is $(PR \text{ x } PR)$ identity matrix. Hence, to display the *J* parts observed in *K* occasions in a *Q*-orthonormal subspace of $\Re^{IK}$, the principal coordinates of parts are $\hat{\mathbf{B}}$ with $\hat{\mathbf{B}} = \mathbf{B}\left(\mathbf{T}_B^t\right)^{-1}$ and $\hat{\mathbf{W}}_B = \mathbf{W}_B\mathbf{T}_B$ is the orthogonal base, where the transformation $\mathbf{T}_B$ matrix is again given by a Gram-Schmidt orthonormalization.

In this form, as known covariance form, the *J* parts are generally plotted as arrows. And due to constrain $\hat{\mathbf{1}}_J\mathbf{B} = \hat{\mathbf{0}}_Q$, the centre of plot is coincident with the centroid of the parts. However, to bring the solution onto the scale of logratio variance and covariance, the principal coordinates have been rescaled by the constant $1/\sqrt{IK-1}$, thus the length of each arrow is an approximation of the standard deviation of the corresponding parts observed into *K* different occasions. In other words, the length of each arrow is an approximated measure of the standard deviation for each row vector of $\mathbf{Y}_B$.

Unfortunately, this measure vary when a subcomposition is considered, because depend on the full composition through the geometrical mean $g\left(\mathbf{v}_i^k\right)$ $(i = 1,\ldots,I;\ k = 1,\ldots,K)$. Thus, in this plot

then we will call *relative variation parts plot*, only the difference between the parts can be considered. The $J(J-1)/2$ differences between the end points of each arrow, called links by Aitchison and Greenacre (2002), indicate the standard deviations of logratio between the parts. Thus, the largest link between two parts indicates the most relative variation, when one arrow is placed on top of another, means that the logratio between these parts is approximately constant. Moreover, links provide information on the correlation between the logratios, it is used to identify subcompositions. In fact, the angle cosine between two links is an approximation of the correlation between the correspondent logratios. Nevertheless, because the point where one link intersect another ones can be not presented into plot, reading the correlation between two links can be a very hard operation. In these cases, it is possible plotting directly the pairwise logratios. In fact, we can observe than the matrix $\hat{\mathbf{B}}$ gives the principal coordinates of parts in case of centred logratios and it is shown than $\mathbf{B} = \mathbf{E}_J \mathbf{M} / \sqrt{J}$ where $\mathbf{E}_J$ is a $\left(J \text{ x } J(J-1)/2\right)$ matrix with 0s in each column except for a 1 and -1 in two rows, and $\mathbf{M}$ is the left singular vectors matrix of the pairwise logratios (see Appendix B for full details).

Hence, the results of analysis of the larger flatted array of pairwise logratios can be obtained from the analysis of to smaller array of the centred logratios data. In fact, it is possible to get the principal coordinates of the pairwise logratios $\tilde{\mathbf{B}}$ by the principal coordinates of the centred logratios $\hat{\mathbf{B}}$: $\tilde{\mathbf{B}} = \sqrt{J}\mathbf{E}_J^t \hat{\mathbf{B}}$. In this case, the $J(J-1)/2$ arrows are the correspondent links and the point of intersection between all the links (arrows) is the centre of plot, while the length of the arrows give the values, in logratio, of the standard deviations.

6. Application

To illustrate how each single mode plot should be interpreted, we consider 'hongite' , 'kongite', 'boxite' and 'coxite' datasets (Aitchison, 1986). The data are arranged in three-way array where each horizontal slice has the percentages by weight of 'albite', 'blandite', 'cornite', 'daubite' and 'endite' observed on 25 specimens of the mineral. These data are *clr* transformed and centred by parts too. Once, double centred the three-way array the principal coordinates for the four objects and the five parts are computed and the relative low-dimensional plots for the $\Re^{80}$ and $\Re^{100}$ are built, respectively, where the first two axis are used for both one mode plots. Differently, the low-dimensional plot for the 25 specimens is not considered here, because they are just a replication of the measure. Thus, for this analysis Tucker2 model with two dimension for each mode are used $(P = Q = 2)$, as the model is able to explain the 76.6% of variability (44.19% and 32.42% for first and second axis, respectively).

In Figure 1.a the distances between the four points are approximations of the distances between the minerals, where the points are centred at the origin of the display and the distance between the points, in this low-dimensional plot, are approximations of the distances between the objects in the original high-dimensional space. Specifically, across the 25 specimens it is possible said than, in term of parts, the compositions of 'boxite' and 'coxite' are more similar to the compositions of 'hongite' and 'kongite'.

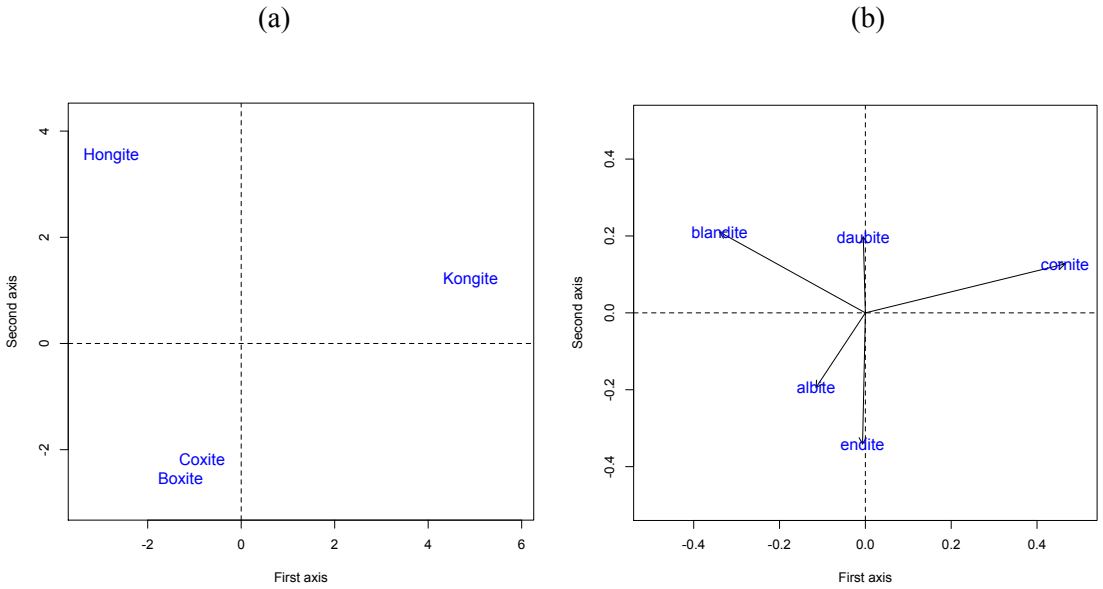

Figure 1: Objects plot (a) and relative variation parts plot (b).

In Figure 1.b, the length of arrows give information on the standard deviation of the correspondent centred logratio, thus it is possible observe than 'blandite' and 'cornite' have a more large standard deviation of 'albite', 'daubite' and 'endite'. But these measures depend on the full composition through the geometrical mean then they are not subcomposition coherence. For this reason only links between the arrows are considered. Each link gives, in term of standard deviation of the logratio, information on the relative variation between the parts. Here can be observed than the variation between 'blandite' and 'endite' is larger than the variation between 'blandite' and 'daubite'.

In term of angle cosine between the links can be verified the highest correlation between 'blandite/cornite' and 'blandite/daudite' or the lowest between 'albite/cornite' and 'daudite/endite'. The correlation between the logratios is more evident in Figure 2. In this plot all links intersect the origin thus the cosines between the arrows are the approximation of correlation and the length of arrows are the approximation of standard deviation of logratios. Thus, 'blandite/cornite' has very high direct correlation with 'blandite/daudite' and very high inverse corrlation with 'albite/blandite'

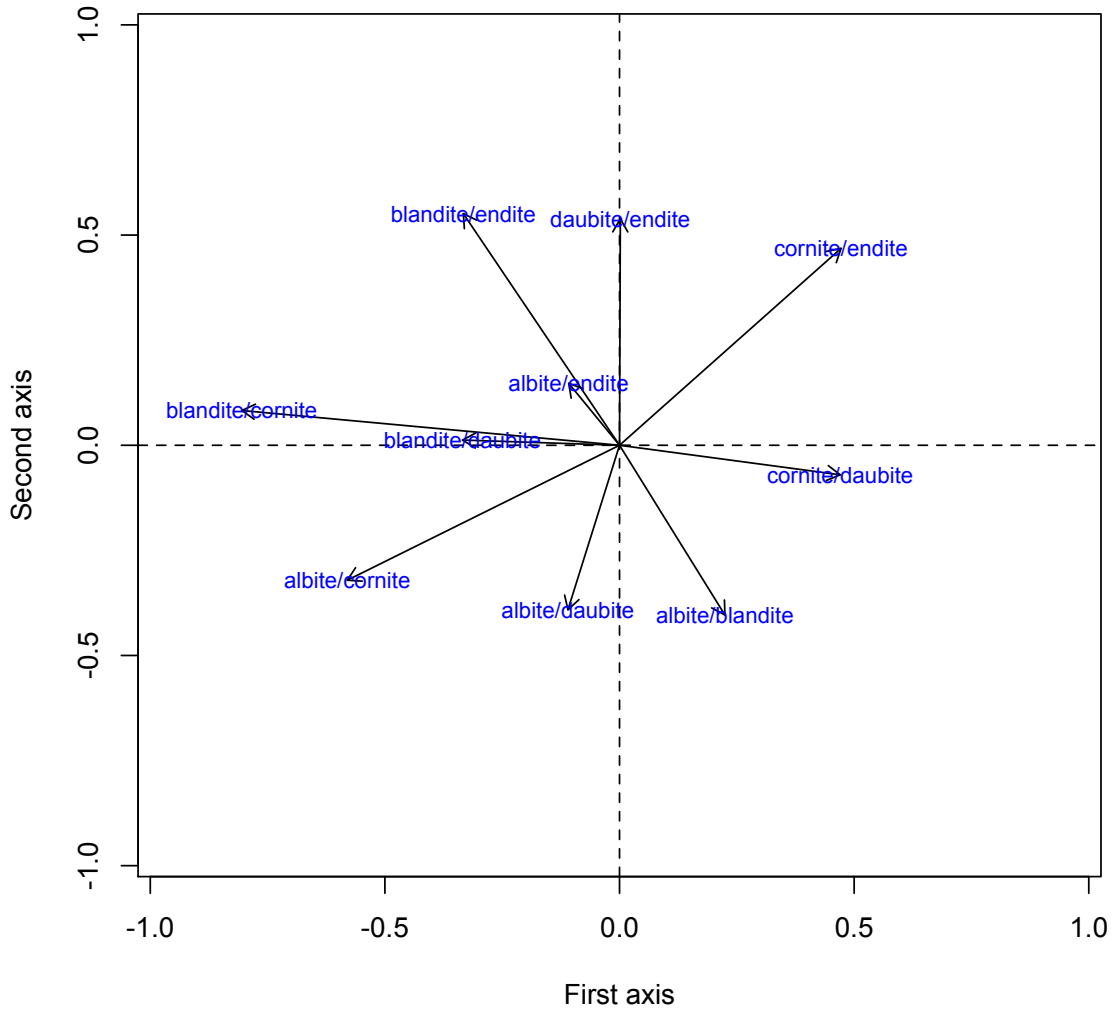

Figure 2: Pairwise logratios parts plot.

7. Conclusion

Through this paper we have shown how three-way array of compositional data can be analyzed by Tucker models and illustrated by one mode plots. The approach is based on the centred logratios transformation of the compositional data and the basic conclusion is that Tucker models give results than satisfy all the properties researched in case of compositional data.

The plotting procedure described here is a very powerful and friend tool for visualizing the Tucker results. In fact, the graphical interpretation of principal components is more easy and intuitive than read the table of values especially when there are more objects and parts. Of course, the distance, the relative variation and the correlation give in these plots are an approximation of the original, and when the plot are inspected should be careful to the percentage of variability explained.

In many cases plotting the occasions can be given very important informations on the variability generate by the third mode. For example, in case of the compositions are measured by different instruments, analyzed by several methods, in several time or geographical position. But in other cases the occasions are just a replication of the measure, e.g. in application, thus we need not to analyze them and Tucker2 model can be used more efficiently. Regarding to Tucker1 model, it is rarely applicable in case of compositional data because the parts are not considered, thus it is studied in this paper just to consider all the family of Tucker models.

Other graphical representation of Tucker results are been proposed, as *relative variation joint biplot* (Gallo, 2011). This is preferable to one mode plots when we would investigate the relationship between the elements of different modes. Thus, plotting together compositions and parts may highlight the relation between them for each occasions. Information than cannot be given by the one mode plots. However, the principal difficulty of *relative variation joint biplot* is the large set of information than can be extracted by it, thus it can not be friend to inspect especially when the dataset presents more parts. In fact, in short, to examine the interpretation principles of *relative variation joint biplot* we can consider than it stays to three-way analysis as the relative joint biplot (Aitchison and Grenacre, 2002) stays to two-way analysis.

Regarding the rebuild of the three-way array of original data, it is well known the *clr* transformation has an inverse function $\left(clr^{-1}\right)$ then if we know the geometrical mean of each compositional vector and the mean for each parts in the different occasions it is possible rebuild the array of original data. Moreover, it is possible get an approximate rebuild of the array of compositional data $\underline{\mathbf{Y}}$ if the loading matrices $\mathbf{A}$,$\mathbf{B}$, $\mathbf{C}$ and the core-array $\underline{\mathbf{G}}$ are known, e.g. the flatted matrix $\hat{\mathbf{Y}}_A$ $\left(\mathbf{Y}_A = \hat{\mathbf{Y}}_A + \mathbf{E}_A\right)$ as $\hat{\mathbf{Y}}_A = \mathbf{A}\mathbf{G}_A\left(\mathbf{C}^t \otimes \mathbf{B}^t\right)$. Unfortunately, in the one mode plots the objects, parts and occasions are displayed as principal components then we can not to have the loading matrices because their values are confused with the transformation matrices used to assure orthonormal axis. Thus, if they are available just one mode plots we can not rebuild the original data.

Appendix A: Geometry for a vector of juxtaposed compositions

Let $\underline{\mathbf{v}}_i = \left[\mathbf{v}_i^1 | \ldots | \mathbf{v}_i^K\right]$ be a vector with the coordinate of *i*th object into K different simplex spaces, where $\mathbf{v}_i^k \in S_k^J$. To have a linear vector space structure for this vector we define perturbation operation, power transformation, inner product, norm and distance.

a. Given the pertubation between two compositions $\mathbf{v}_i^k, \mathbf{v}_{i'}^k \in S_k^J$:

$\mathbf{v}_i^k \oplus \mathbf{v}_{i'}^k = \mathbb{C}\left[v_{i1k}v_{i'1k}, \ldots, v_{ijk}v_{i'jk}, \ldots, v_{iJk}v_{i'Jk}\right]$; then the perturbation between $\underline{\mathbf{v}}_i$ and $\underline{\mathbf{v}}_{i'}$ is

$\underline{\mathbf{v}}_i \oplus \underline{\mathbf{v}}_{i'} = \left[\mathbb{C}\left[v_{i11}v_{i'11}, \ldots, v_{iJ1}v_{i'J1}\right] | \ldots | \mathbb{C}\left[v_{i1k}v_{i'1k}, \ldots, v_{iJk}v_{i'Jk}\right] | \ldots | \mathbb{C}\left[v_{i1K}v_{i'1K}, \ldots, v_{iJk}v_{i'JK}\right]\right]$

b. Given the power transformation of a composition vector $\mathbf{v}_i^k \in S_k^J$ by a constant $\alpha \in \Re$:

$\alpha \odot \mathbf{v}_i^k = \mathbb{C}\left[v_{i1k}^\alpha, \ldots, v_{ijk}^\alpha, \ldots, v_{iJk}^\alpha\right]$; then the power of $\underline{\mathbf{v}}_i$ by a constant $\alpha \in \Re$ is

$\alpha \odot \underline{\mathbf{v}}_i = \left[\mathbb{C}\left[v_{i11}^\alpha, \ldots, v_{iJ1}^\alpha\right] | \ldots | \mathbb{C}\left[v_{i1k}^\alpha, , \ldots, v_{iJk}^\alpha\right] | \ldots | \mathbb{C}\left[v_{i1K}^\alpha, \ldots, v_{iJK}^\alpha\right]\right]$

c. Given the inner product between two compositions $\mathbf{v}_i^k, \mathbf{v}_{i'}^k \in S_k^J$:

$\left\langle \mathbf{v}_i^k, \mathbf{v}_{i'}^k \right\rangle_\alpha = \sum_{j=1}^{J}\sum_{j'=1}^{J} \log\left(\mathrm{v}_{ijk} / \mathrm{v}_{ij'k}\right)\log\left(\mathrm{v}_{i'jk} / \mathrm{v}_{i'j'k}\right) / 2J$; then the inner product between $\underline{\mathbf{v}}_i$ and $\underline{\mathbf{v}}_{i'}$ is

$$\left\langle \underline{\mathbf{v}}_i, \underline{\mathbf{v}}_{i'} \right\rangle_\alpha = \sum_{k=1}^{K}\sum_{j=1}^{J}\sum_{j'=1}^{J} \log\left(\mathrm{v}_{ijk} / \mathrm{v}_{ij'k}\right)\log\left(\mathrm{v}_{i'jk} / \mathrm{v}_{i'j'k}\right) / 2JK$$

d. Given the norm of $\mathbf{v}_i^k \in S_k^J$: $\left\|\mathbf{v}_i^k\right\|_\alpha = \left[\sum_{j=1}^{J}\sum_{j'=1}^{J} \log\left(\mathrm{v}_{ijk} / \mathrm{v}_{ij'k}\right)^2 / 2J\right]^{1/2}$; then the norm of $\underline{\mathbf{v}}_i$ is

$$\left\|\underline{\mathbf{v}}_i\right\|_\alpha = \left[\sum_{k=1}^{K}\sum_{j=1}^{J}\sum_{j'=1}^{J} \log\left(\mathrm{v}_{ijk} / \mathrm{v}_{ij'k}\right)^2 / 2JK\right]^{1/2}$$

e. Given the distance between two compositions $\mathbf{v}_i^k, \mathbf{v}_{i'}^k \in S_k^J$:

$d_\alpha\left(\mathbf{v}_i^k, \mathbf{v}_{i'}^k\right) = \left[\sum_{j=1}^{J}\sum_{j'=1}^{J}\left(\log\left(\mathrm{v}_{ijk} / \mathrm{v}_{ij'k}\right) - \log\left(\mathrm{v}_{i'jk} / \mathrm{v}_{i'j'k}\right)\right)^2 / 2J\right]^{1/2}$; then the distance between $\underline{\mathbf{v}}_i$ and $\underline{\mathbf{v}}_{i'}$ is $d_\alpha\left(\underline{\mathbf{v}}_i, \underline{\mathbf{v}}_{i'}\right) = \left[\sum_{k=1}^{K}\sum_{j=1}^{J}\sum_{j'=1}^{J}\left(\log\left(\mathrm{v}_{ijk} / \mathrm{v}_{ij'k}\right) - \log\left(\mathrm{v}_{i'jk} / \mathrm{v}_{i'j'k}\right)\right)^2 / 2JK\right]^{1/2}$.

Thus, this structure satisfies the following properties:

a. $d_\alpha\left(\underline{\mathbf{v}}_i, \underline{\mathbf{v}}_{i'}\right) = d_\alpha\left(\underline{\mathbf{v}}_{i''} \oplus \underline{\mathbf{v}}_i, \underline{\mathbf{v}}_{i''} \oplus \underline{\mathbf{v}}_{i'}\right)$

b. $|\alpha| d_\alpha\left(\underline{\mathbf{v}}_i, \underline{\mathbf{v}}_{i'}\right) = d_\alpha\left(\alpha \odot \underline{\mathbf{v}}_i, \alpha \odot \underline{\mathbf{v}}_{i'}\right)$

Appendix B: Equivalence of logratio and centred logratio plot of first and second mode

Let $\mathbf{L}$ $(I \text{ x } J \text{ x } K)$ be an array with typical element $\log\left(v_{ijk}\right)$, and $\mathbf{L}_k$ the kth frontal slice $(k = 1,...,K)$. Given $\mathbf{P}_J^\perp = \left(\mathbf{I}_J - \hat{\mathbf{1}}_J \hat{\mathbf{1}}_J^t / J\right)$ the symmetric and idempotent centring matrix, the kth frontal slice of the centred logratios can be write $\mathbf{L}_k \mathbf{P}_J^\perp$ with typical element $clr\left(\mathrm{v}_{ijk}\right) = \log\left(v_{ijk} / g\left(\mathbf{v}_i^k\right)\right) = \log\left(v_{ijk}\right) - (1/J)\sum_j \log(v_{ijk})$. Thus, for the kth frontal slice, the double centred logratios matrix is $\mathbf{Y}_k = \mathbf{P}_I^\perp \mathbf{L}_k \mathbf{P}_J^\perp$. Let $\mathbf{E}_J$ be a $\left(J \text{ x } J(J-1)/2\right)$ matrix with 0s in each column except for a 1 and -1 in two rows, since $\mathbf{E}_J \mathbf{E}_J^t = J\mathbf{P}_J^\perp$. Thus, the typical element of $\mathbf{L}_k \mathbf{E}_J$ is the pairwise logratios $\log\left(v_{ijk} / v_{ij'k}\right)$, and $\mathbf{X}_k = \mathbf{P}_I^\perp \mathbf{L}_k \mathbf{E}_J$ is the kth pairwise logratios frontal slice, again centred with respect to column.

To verify the equivalence between pairwise and centred logratios for first - and second-mode, the SVD of $\mathbf{Y}_A = \left[\mathbf{Y}_1 \ldots \mathbf{Y}_k \ldots \mathbf{Y}_K\right]$, $\mathbf{Y}_B = \left[\mathbf{Y}_1^t \ldots \mathbf{Y}_k^t \ldots \mathbf{Y}_K^t\right]$, $\mathbf{X}_A = \left[\mathbf{X}_1 \ldots \mathbf{X}_k \ldots \mathbf{X}_K\right]$ and $\mathbf{X}_B = \left[\mathbf{X}_1^t \ldots \mathbf{X}_k^t \ldots \mathbf{X}_K^t\right]$ are considered, where the rank of all flatted matrices is equal F.

1. Equivalence of pairwise and centred logratio plot for first mode

Suppose that $\mathbf{Y}_A$ has SVD $\mathbf{Y}_A = \mathbf{U}_{I \text{ x } F} \Gamma_{F \text{ x } F} \mathbf{V}_{F \text{ x } JK}^t$ and $\mathbf{X}_A$ has SVD $\mathbf{X}_A = \mathbf{M}_{I \text{ x } F} \Psi_{F \text{ x } F} \mathbf{N}_{F \text{ x } J(J-1)K/2}^t$ then the left singular vectors are identical: $\mathbf{M} = \mathbf{U}$; while the singular values differ by the constant factor $\sqrt{J}$: $\Psi = \sqrt{J}\Gamma$.

proof:

$$\mathbf{Y}_A \mathbf{Y}_A^t = \left[\mathbf{Y}_1 | \ldots | \mathbf{Y}_k | \ldots | \mathbf{Y}_k\right]\left[\mathbf{Y}_1 | \ldots | \mathbf{Y}_k | \ldots | \mathbf{Y}_k\right]^t = \left[\mathbf{Y}_1\mathbf{Y}_1^t | \ldots | \mathbf{Y}_k\mathbf{Y}_k^t | \ldots | \mathbf{Y}_K\mathbf{Y}_K^t\right]$$

$$= \left[\mathbf{P}_I^{\perp}\mathbf{L}_1\mathbf{P}_J^{\perp}\mathbf{P}_J^{\perp}\mathbf{L}_1^t\mathbf{P}_I^{\perp}|\ldots|\mathbf{P}_I^{\perp}\mathbf{L}_k\mathbf{P}_J^{\perp}\mathbf{P}_J^{\perp}\mathbf{L}_k^t\mathbf{P}_I^{\perp}|\ldots|\mathbf{P}_I^{\perp}\mathbf{L}_K\mathbf{P}_J^{\perp}\mathbf{P}_J^{\perp}\mathbf{L}_K^t\mathbf{P}_I^{\perp}\right]$$

$$= \left[\mathbf{P}_I^{\perp}\mathbf{L}_1\mathbf{P}_J^{\perp}\mathbf{L}_1^t\mathbf{P}_I^{\perp}|\ldots|\mathbf{P}_I^{\perp}\mathbf{L}_k\mathbf{P}_J^{\perp}\mathbf{L}_k^t\mathbf{P}_I^{\perp}|\ldots|\mathbf{P}_I^{\perp}\mathbf{L}_K\mathbf{P}_J^{\perp}\mathbf{L}_K^t\mathbf{P}_I^{\perp}\right]$$

$$= \mathbf{P}_I^{\perp}\left[\mathbf{L}_1\mathbf{P}_J^{\perp}\mathbf{L}_1^t|\ldots|\mathbf{L}_k\mathbf{P}_J^{\perp}\mathbf{L}_k^t|\ldots|\mathbf{L}_K\mathbf{P}_J^{\perp}\mathbf{L}_K^t\right]\mathbf{P}_I^{\perp} = \mathbf{P}_I^{\perp}\mathbf{U}\Gamma^2\mathbf{U}^t\mathbf{P}_I^{\perp}$$

$$\mathbf{X}_A\mathbf{X}_A^t = \left[\mathbf{X}_1|\ldots|\mathbf{X}_k|\ldots|\mathbf{X}_K\right]\left[\mathbf{X}_1^t|\ldots|\mathbf{X}_k^t|\ldots|\mathbf{X}_K^t\right]^t = \left[\mathbf{X}_1\mathbf{X}_1^t|\ldots|\mathbf{X}_k\mathbf{X}_k^t|\ldots|\mathbf{X}_K\mathbf{X}_K^t\right]$$

$$= \left[\mathbf{P}_I^{\perp}\mathbf{L}_1\mathbf{E}_1\mathbf{E}_1^t\mathbf{L}_1^t\mathbf{P}_I^{\perp}|\ldots|\mathbf{P}_I^{\perp}\mathbf{L}_k\mathbf{E}_k\mathbf{E}_k^t\mathbf{L}_k^t\mathbf{P}_I^{\perp}|\ldots|\mathbf{P}_I^{\perp}\mathbf{L}_K\mathbf{E}_K\mathbf{E}_K^t\mathbf{L}_K^t\mathbf{P}_I^{\perp}\right]$$

$$= \left[\mathbf{P}_I^{\perp}\mathbf{L}_1J\mathbf{P}_J^{\perp}\mathbf{L}_1^t\mathbf{P}_I^{\perp}|\ldots|\mathbf{P}_I^{\perp}\mathbf{L}_kJ\mathbf{P}_J^{\perp}\mathbf{L}_k^t\mathbf{P}_I^{\perp}|\ldots|\mathbf{P}_I^{\perp}\mathbf{L}_KJ\mathbf{P}_J^{\perp}\mathbf{L}_K^t\mathbf{P}_I^{\perp}\right]$$

$$= \mathbf{P}_I^{\perp}\left[\mathbf{L}_1J\mathbf{P}_J^{\perp}\mathbf{L}_1^t|\ldots|\mathbf{L}_kJ\mathbf{P}_J^{\perp}\mathbf{L}_k^t|\ldots|\mathbf{L}_KJ\mathbf{P}_J^{\perp}\mathbf{L}_K^t\right]\mathbf{P}_I^{\perp} = \mathbf{P}_I^{\perp}\mathbf{U}JK\Gamma^2\mathbf{U}^t\mathbf{P}_I^{\perp}$$

2. Equivalence of pairwise and centred logratio plot for second mode

Suppose that $\mathbf{Y}_B$ has SVD $\mathbf{Y}_B = \mathbf{U}_{J,F}\Gamma_{F,F}\mathbf{V}_{F,IK}^t$ and $\mathbf{X}_B$ has SVD $\mathbf{X}_B = \mathbf{M}_{J(J-1)K/2,F}\Psi_{F,F}\mathbf{N}_{F,IK}^t$ then $\mathbf{Y}_B\mathbf{Y}_B^t = \mathbf{P}_J^{\perp}\mathbf{U}\Gamma^2\mathbf{U}^t\mathbf{P}_J^{\perp}$ and $\mathbf{X}_B\mathbf{X}_B^t = \mathbf{E}_J^t\mathbf{U}\Gamma^2\mathbf{U}^t\mathbf{E}_J$, since $\mathbf{U}^t\mathbf{E}_J\mathbf{E}_J^t\mathbf{U} = \mathbf{U}^tJ\mathbf{P}_J^{\perp}\mathbf{U} = J\mathbf{I}$ then between the left singular vectors there are the follow relation $\mathbf{M} = \mathbf{E}^t\mathbf{U}/\sqrt{J}$; while the singular values differ by the constant factor $\sqrt{J}$: $\Psi = \sqrt{J}\Gamma$.

proof:

$$\mathbf{Y}_B\mathbf{Y}_B^t = \left[\mathbf{Y}_1^t\ldots\mathbf{Y}_k^t\ldots\mathbf{Y}_K^t\right]\left[\mathbf{Y}_1^t\ldots\mathbf{Y}_k^t\ldots\mathbf{Y}_K^t\right]^t = \left[\mathbf{Y}_1^t\left(\mathbf{Y}_1^t\right)^t\ldots\mathbf{Y}_k^t\left(\mathbf{Y}_k^t\right)^t\ldots\mathbf{Y}_K^t\left(\mathbf{Y}_K^t\right)^t\right]$$

$$= \left[\mathbf{P}_J^{\perp}\mathbf{L}_1^t\mathbf{P}_I^{\perp}\mathbf{P}_I^{\perp}\mathbf{L}_1\mathbf{P}_J^{\perp}|\ldots|\mathbf{P}_J^{\perp}\mathbf{L}_k^t\mathbf{P}_I^{\perp}\mathbf{P}_I^{\perp}\mathbf{L}_k\mathbf{P}_J^{\perp}|\ldots|\mathbf{P}_J^{\perp}\mathbf{L}_K^t\mathbf{P}_I^{\perp}\mathbf{P}_I^{\perp}\mathbf{L}_K\mathbf{P}_J^{\perp}\right]$$

$$= \left[\mathbf{P}_J^{\perp}\mathbf{L}_1^t\mathbf{P}_I^{\perp}\mathbf{L}_1\mathbf{P}_J^{\perp}|\ldots|\mathbf{P}_J^{\perp}\mathbf{L}_k^t\mathbf{P}_I^{\perp}\mathbf{L}_k\mathbf{P}_J^{\perp}|\ldots|\mathbf{P}_J^{\perp}\mathbf{L}_K^t\mathbf{P}_I^{\perp}\mathbf{L}_K\mathbf{P}_J^{\perp}\right]$$

$$= \mathbf{P}_J^{\perp}\left[\mathbf{L}_1^t\mathbf{P}_I^{\perp}\mathbf{L}_1|\ldots|\mathbf{L}_k^t\mathbf{P}_I^{\perp}\mathbf{L}_k|\ldots|\mathbf{L}_K^t\mathbf{P}_I^{\perp}\mathbf{L}_K\right]\mathbf{P}_J^{\perp} = \mathbf{P}_J^{\perp}\mathbf{U}\Gamma^2\mathbf{U}^t\mathbf{P}_J^{\perp}$$

$$\mathbf{X}_B\mathbf{X}_B^t = \left[\mathbf{X}_1^t|\ldots|\mathbf{X}_k^t|\ldots|\mathbf{X}_K^t\right]\left[\mathbf{X}_1^t|\ldots|\mathbf{X}_k^t|\ldots|\mathbf{X}_K^t\right]^t = \left[\mathbf{X}_1^t\left(\mathbf{X}_1^t\right)^t|\ldots|\mathbf{X}_k^t\left(\mathbf{X}_k^t\right)^t|\ldots|\mathbf{X}_K^t\left(\mathbf{X}_K^t\right)^t\right]$$

$$= \left[\mathbf{E}_J^t\mathbf{L}_1^t\mathbf{P}_I^{\perp}\mathbf{P}_I^{\perp}\mathbf{L}_1\mathbf{E}_J|\ldots|\mathbf{E}_J^t\mathbf{L}_k^t\mathbf{P}_I^{\perp}\mathbf{P}_I^{\perp}\mathbf{L}_k\mathbf{E}_J|\ldots|\mathbf{E}_J^t\mathbf{L}_K^t\mathbf{P}_I^{\perp}\mathbf{P}_I^{\perp}\mathbf{L}_K\mathbf{E}_J\right]$$

$$= \left[\mathbf{E}_J^t\mathbf{L}_1^t\mathbf{P}_I^{\perp}\mathbf{L}_1\mathbf{E}_J|\ldots|\mathbf{E}_J^t\mathbf{L}_k^t\mathbf{P}_I^{\perp}\mathbf{L}_k\mathbf{E}_J|\ldots|\mathbf{E}_J^t\mathbf{L}_K^t\mathbf{P}_I^{\perp}\mathbf{L}_K\mathbf{E}_J\right] = \mathbf{E}_J^t\left[\mathbf{L}_1^t\mathbf{P}_I^{\perp}\mathbf{L}_1|\ldots|\mathbf{L}_k^t\mathbf{P}_I^{\perp}\mathbf{L}_k|\ldots|\mathbf{L}_K^t\mathbf{P}_I^{\perp}\mathbf{L}_K\right]\mathbf{E}_J$$

$$= \mathbf{E}_J^t\mathbf{U}\Gamma^2\mathbf{U}^t\mathbf{E}_J$$

It follow that the coordinates for the $J(J-1)/2$ pairwise logratios, $\mathbf{X}_B$, can be given determinate by the Tucker3 analysis of $\mathbf{Y}_B$. Specifically, the coordinates for the $J(J-1)/2$ pairwise logratios are $\hat{\mathbf{B}} = \sqrt{J}\mathbf{E}_J\mathbf{B}\mathbf{G}_B$ and they can be plotted on orthonormal basis $\hat{\mathbf{W}}_B^t = \left(\mathbf{C}^t \otimes \mathbf{A}^t\right)$.

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