TCA and TLRA: A comparison on contingency tables and compositional data

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Abstract

There are two popular general approaches for the analysis and visualization of a contingency table and a compositional data set: Correspondence analysis (CA) and log ratio analysis (LRA). LRA includes two independently well developed methods: association models and compositional data analysis. The application of either CA or LRA to a contingency table or to compositional data set includes a preprocessing centering step. In CA the centering step is multiplicative, while in LRA it is log bi-additive. A preprocessed matrix is double-centered, so it is a residuel matrix; which implies that it affects the final results of the analysis. This paper introduces a novel index named the intrinsic measure of the quality of the signs of the residuals (QSR) for the choice of the preprocessing, and consequently of the method. The criterion is based on taxicab singular value decomposition (TSVD) on which the package TaxicabCA in R is developed. We present a minimal R script that can be executed to obtain the numerical results and the maps in this paper. Three relatively small sized data sets available freely on the web are used as examples.

Key words: Taxicab SVD; correspondence analysis; log ratio analysis; CODA; association model; QSR index.

AMS 2010 subject classifications: 62H25, 62H30
1 Introduction

There are two popular general approaches for the analysis and visualization of a contingency table or a compositional data set: Correspondence analysis (CA) and log ratio analysis (LRA). LRA includes two independently well developed methods: RC association models by Goodman (1991, 1996) and compositional data analysis (CODA) by Aitchison (1986). Correspondence analysis and log-ratio related methods are based on different invariance principles: CA on Benzécri’s distributional equivalence principle, RC association models on Yule’s scale invariance principle, and CODA on Aitchison’s subcompositional coherence principle. RC and CODA are mathematically speaking identical. Each of the method, CA or LRA, includes a preprocessing-centering step of the data set. In CA the preprocessing step is multiplicative, while in LRA it is log bi-additive. A preprocessed contingency table or a compositional set is double-centered, so it is a residual matrix which affects the subsequent computations. Our aim is to introduce a simple intuitive criterion for the choice of the preprocessing, and consequently of the method. The novel criterion is the intrinsic measure of quality of the signs of the residuals (QSR) by a principal dimension. For each principal dimension QSR is calculated via taxicab singular value decomposition (TSVD) on which the package TaxicabCA in R is developed. TaxicabCA in R is developed by Allard and Choulakian (2019). Three relatively small data sets, two contingency tables and one compositional data set, available freely on the web are used to explain the use of the package for the choice of the best method between taxicab CA (TCA) or taxicab LRA (TLRA). The reference for correspondance analysis is Benzécri (1973). For a panoramic review of CA and its variants, see Beh and Lombardo (2014).

This paper is organized as follows. In Section 2, we present an overview of taxicab singular value decomposition (TSVD) and in Section 3, the computation pertaining to the methods TCA and TLRA. Section 4 presents the QSR index. In Section 5, we present three examples and their analyses. In Section 6, we present a minimal R script that can be executed to obtain the numerical results and the maps in this paper. Finally, we conclude in Section 7.
2 An overview of taxicab singular value decomposition

Consider a matrix $X$ of size $I \times J$ and $\text{rank}(X) = k$. Taxicab singular value decomposition (TSVD) of $X$ is a decomposition similar to SVD($X$), see Choulakian (2006, 2016).

In TSVD the calculation of the dispersion measures ($\delta_\alpha$), principal axes ($u_\alpha, v_\alpha$) and principal scores ($a_\alpha, b_\alpha$) for $\alpha = 1, \ldots, k$ is done in a stepwise manner. We put $X_1 = X = (x_{ij})$ and $X_\alpha$ the residual matrix at the $\alpha$-th iteration for $\alpha = 1, \ldots, k$.

The variational definitions of the TSVD at the $\alpha$-th iteration are

$$
\delta_\alpha = \max_{u \in \mathbb{R}^J} \frac{||X_\alpha u||_1}{||u||_\infty} = \max_{v \in \mathbb{R}^I} \frac{||X_\alpha' v||_1}{||v||_\infty} = \max_{u \in \mathbb{R}^J, v \in \mathbb{R}^I} \frac{v'X_\alpha u}{||u||_\infty ||v||_\infty},
$$

$$
= \max ||X_\alpha u||_1 \text{ subject to } u \in \{-1,+1\}^J,
$$

$$
= \max ||X_\alpha' v||_1 \text{ subject to } v \in \{-1,+1\}^I,
$$

$$
= \max v'X_\alpha u \text{ subject to } u \in \{-1,+1\}^J, v \in \{-1,+1\}^I.
$$

(1)

The $\alpha$-th principal axes are

$$
u_\alpha = \arg \max_{u \in \{-1,+1\}^J} ||X_\alpha u||_1 \text{ and } v_\alpha = \arg \max_{v \in \{-1,+1\}^I} ||X_\alpha' v||_1,
$$

(2)

and the $\alpha$-th principal projections of the rows and the columns are

$$
a_\alpha = X_\alpha u_\alpha \text{ and } b_\alpha = X_\alpha' v_\alpha.
$$

(3)

Furthermore, the following relations are also useful

$$
u_\alpha = \text{sign}(b_\alpha) \text{ and } v_\alpha = \text{sign}(a_\alpha),
$$

(4)

where $\text{sign}(.)$ is the coordinatewise sign function, $\text{sign}(x) = 1$ if $x > 0$, and $\text{sign}(x) = -1$ if $x \leq 0$.

The $\alpha$-th taxicab dispersion measure $\delta_\alpha$ can be represented in many different ways

$$
\delta_\alpha = ||X_\alpha u_\alpha||_1 = ||a_\alpha||_1 = a_\alpha' v_\alpha,
$$

$$
= ||X_\alpha' v_\alpha||_1 = ||b_\alpha||_1 = b_\alpha' u_\alpha.
$$

(5)
The \((\alpha + 1)\)-th residual matrix is

\[ X_{\alpha+1} = X_{\alpha} - a_{\alpha} b'_{\alpha} / \delta_{\alpha}. \] (6)

An interpretation of the term \(a_{\alpha} b'_{\alpha} / \delta_{\alpha}\) in (6) is that, it represents the best rank-1 approximation of the residual matrix \(X_{\alpha}\), in the sense of the taxicab matrix norm (1).

Thus TSVD(\(X\)) corresponds to the bilinear decomposition

\[ x_{ij} = \sum_{\alpha=1}^{k} a_{\alpha}(i) b_{\alpha}(j) / \delta_{\alpha}, \] (7)

a decomposition similar to SVD, but where the vectors \((a_{\alpha}, b_{\alpha})\) for \(\alpha = 1, ..., k\) are conjugate, that is

\[ a'_{\alpha} v_{\beta} = a'_{\alpha} \text{sign}(a_{\beta}) = b'_{\alpha} u_{\beta} = b'_{\alpha} \text{sign}(b_{\beta}) = 0 \text{ for } \beta \geq \alpha + 1. \] (8)

In the package TaxicabCA in R, the calculation of the principal component weights, \(u_{\alpha}\) and \(v_{\alpha}\), are accomplished by three algorithms. The first one, based on complete enumeration equation (2), is named exhaustive. The second one, based on iterating the transition formulae (3,4), is named criss-cross. The third one is based on the genetic algorithm named genetic.

3 TCA and TLRA

Let \(N = (n_{ij})\) be a contingency table or a compositional data set of size \(I \times J\), where \(n_{ij} \geq 0\). Let \(P = N/t = (p_{ij})\) be the associated correspondence matrix, where \(t = \sum_{i=1}^{I} \sum_{j=1}^{J} n_{ij}\). We define as usual \(p_{i*} = \sum_{j=1}^{J} p_{ij}\) and \(p_{*j} = \sum_{i=1}^{I} p_{ij}\) the row and column marginals, respectively. We present the three steps of calculation necessary in TCA and TLRA.

3.1 TCA

Step 1: Center the data:
\[ X_1 = (X_1(i, j)) = (p_{ij} - p_{i*}p_{*j}). \]

Step 2: Calculate TSVD(\(X_1\))

\[ p_{ij} - p_{i*}p_{*j} = \sum_{\alpha=1}^{k} a_{\alpha}(i)b_{\alpha}(j)/\delta_{\alpha}. \]  

Step 3: Calculate TCA(\(P\)) by dividing each term in (10) by \(p_{i*}p_{*j}\)

\[ \frac{p_{ij} - p_{i*}p_{*j}}{p_{i*}p_{*j}} = \sum_{\alpha=1}^{k} f_{\alpha}(i)g_{\alpha}(j)/\delta_{\alpha}, \]

where evidently \(f_{\alpha}(i) = a_{\alpha}(i)/p_{i*}\) and \(g_{\alpha}(j) = b_{\alpha}(j)/p_{*j}\). We name \((a_{\alpha}(i), b_{\alpha}(j))\) TCA contribution scores. Similarly, \((f_{\alpha}(i), g_{\alpha}(j))\) are named TCA principal scores.

### 3.2 TLRA

We obtain TLRA, by weighing each row and column uniformly. Then we proceed according to the following steps:

Step 1: Center the log data \(G_{ij} = \log(p_{ij})\):

\[ X_1(i, j) = G_{ij} - G_{i*} - G_{*j} + G_{**}, \]

where \(G_{i*} = \sum_{j=1}^{J} G_{ij}/J, G_{*j} = \sum_{i=1}^{I} G_{ij}/I\) and \(G_{**} = \sum_{j=1}^{J} \sum_{i=1}^{I} G_{ij}/(IJ)\). This is equation 2.2.1 in Goodman(1991) or equation 5 in Goodman(1996).

Step 2: Calculate TSVD(\(X_1\))

\[ X_1(i, j) = \sum_{\alpha=1}^{k} a_{\alpha}(i)b_{\alpha}(j)/\delta_{\alpha}. \]  

Step 3: Calculate TLRA(\(P\)) by dividing each term in (13) by \(1/(IJ)\)

\[ \frac{G_{ij} - G_{i*} - G_{*j} + G_{**}}{1/(IJ)} = \sum_{\alpha=1}^{k} f_{\alpha}(i)g_{\alpha}(j)/\delta_{\alpha}, \]

where evidently \(f_{\alpha}(i) = I a_{\alpha}(i)\) and \(g_{\alpha}(j) = J b_{\alpha}(j)\). We name \((a_{\alpha}(i), b_{\alpha}(j))\) TLRA contribution scores. Similarly, \((f_{\alpha}(i), g_{\alpha}(j))\) are named TLRA principal scores.
3.3 Facts

Fact 1: In both methods the matrix $X_1 = (X_1(i,j))$ is double-centered

$$\sum_{i=1}^{I} X_1(i,j) = \sum_{j=1}^{J} X_1(i,j) = 0.$$ 

Fact 2: The set of scores $(a_\alpha(i))$ and $(b_\alpha(j))$, besides satisfying (5) and (8) are centered

$$\sum_{i=1}^{I} a_\alpha(i) = \sum_{j=1}^{J} b_\alpha(j) = 0 \quad \text{for } \alpha = 1, ..., k.$$ 

Fact 3: Let $I_1 = \{1, ..., I\}$ and $J_1 = \{1, ..., J\}$; and $S \cup \overline{S} = I_1$ be the partition of $I_1$, and $T \cup \overline{T} = J_1$ be the partition of $J_1$, such that $S = \{i : a_\alpha(i) > 0\}$ and $T = \{j : b_\alpha(j) > 0\}$. $\overline{S}$ and $\overline{T}$ are the complements of $S$ and $T$, respectively. Let also,

$$X_{m+1}(i,j) = X_1(i,j) - \sum_{\alpha=1}^{m} a_\alpha(i)b_\alpha(j)/\delta_\alpha \quad \text{for } m = 1, ..., k - 1,$$

be $(m+1)$th residual matrix. Besides (5), the taxicab dispersion $\delta_m$ will additionally be related to the contribution scores $a_m(i)$ and $b_m(j)$ in (10,14) by the following useful equations, see Choulakian and Abou-Samra (2020):

$$\delta_m/2 = \sum_{i \in S} a_m(i) = -\sum_{i \in \overline{S}} a_m(i) = \sum_{j \in T} b_m(j) = -\sum_{j \in \overline{T}} b_m(j);$$

which tells that the principal dimensions are balanced. Furthermore

$$\delta_m/4 = \sum_{(i,j) \in S \times T} X_m(i,j) = \sum_{(i,j) \in \overline{S} \times \overline{T}} X_m(i,j) = -\sum_{(i,j) \in S \times T} X_m(i,j) = -\sum_{(i,j) \in \overline{S} \times \overline{T}} X_m(i,j);$$
which tells that the $m$th principal dimension divides the residual data matrix $X_m$ into 4 balanced quadrants.

In both methods, the symmetric maps are obtained by plotting $(f_\alpha(i), f_\beta(i))$ or $(g_\alpha(j), g_\beta(j))$ for $\alpha \neq \beta$.

4 Quantifying the intrinsic quality of a taxi-cab principal axis

We briefly review the quality of measures of a principal dimension in the Euclidean framework, then within the Taxicab framework.

4.1 Euclidean framework

Within the Euclidean framework a common used measure of the quality of a principal dimension $\alpha$ of the residual matrix $X_1$ described in (13), is the proportion of variance explained (or inertia in the case of CA)

$$\tau_1(\alpha) = \%	ext{(explained total variance by dimension } \alpha)$$

$$= 100 \frac{\sigma^2_\alpha}{\sum_{\beta=1}^{k} \sigma^2_\beta} \quad \text{for } \alpha = 1, \ldots, k$$

$$= \frac{100 \sigma^2_\alpha}{\sum_{(i,j)} |X_1(i,j)|^2}.$$

Another variant is

$$\tau_2(\alpha) = \%	ext{(explained residual variance by dimension } \alpha)$$

$$= 100 \frac{\sigma^2_\alpha}{\sum_{\beta=\alpha}^{k} \sigma^2_\beta} \quad \text{for } \alpha = \beta, \ldots, k$$

$$= \frac{100 \sigma^2_\alpha}{\sum_{(i,j)} |X_\alpha(i,j)|^2}.$$

Note that $\tau_1(\alpha)$ and $\tau_2(\alpha)$ are extrinsic measures of quality of the residuals in the residual matrix $X_\alpha$, because they compare the intrinsic dispersion of a principal axis $\sigma^2_\alpha$ to the total dispersion $\sum_{\alpha=1}^{k} \sigma^2_\alpha$ or to the partial residual dispersion $\sum_{\beta=\alpha}^{k} \sigma^2_\beta$. Furthermore, when $\tau_1(\alpha)$ and $\tau_2(\alpha)$ are expressed in
proportion, we have the following evident result that should be compared with Lemma 2.

**Lemma 1:**
- a) $1 > \tau_i(\alpha)$ for $i = 1, 2$ and $\alpha = 1, ..., k - 1$.
- b) For $\alpha = k, 1 = \tau_2(\alpha)$.

### 4.2 Taxicab framework

The Taxicab variant of $\tau_2$ is particularly adapted in TSVD

$$QSR_\alpha = \frac{\delta_\alpha}{\sum_{(i,j)} |X_\alpha(i,j)|},$$

which we will interpret as a new intrinsic measure of quality of the signs of the residuals in the residual matrix $X_\alpha$ for $\alpha = 1, ..., k$. As usual $|a|$ designates absolute value of the real number $a$.

Let $S \cup \overline{S} = I_1$ be the optimal principal axis partition of $I_1$, and similarly $T \cup \overline{T} = J_1$ be the optimal principal axis partition of $J_1$, such that $S = \{i : a_\alpha(i) > 0\} = \{i : v_\alpha(i) > 0\}$ and $T = \{j : b_\alpha(j) > 0\} = \{j : u_\alpha(j) > 0\}$ by (4). Thus the data set is divided into four quadrants. Based on the equations (16), we define a new index quantifying the quality of the signs of the residuals in each quadrant of the $\alpha$th residual matrix $X_\alpha$ for $\alpha = 1, ..., k$.

**Definition:** For $\alpha = 1, ..., k - 1$, an intrinsic measure of the quality of the signs of the residuals in the quadrant $E \times F \subseteq I_1 \times J_1$ is

$$QSR_\alpha(E, F) = \frac{\sum_{(i,j) \in E \times F} X_\alpha(i,j)}{\sum_{(i,j) \in E \times F} |X_\alpha(i,j)|} = \frac{\delta_\alpha/4}{\sum_{(i,j) \in E \times F} |X_\alpha(i,j)|},$$

for $E = S$ and $\overline{S}$, and, $F = T$ and $\overline{T}$. The second right-hand side in the above equation derives from equation (16).

We have the following easily proved
Lemma 2: a) For $\alpha = 1, \ldots, k-1$, $QSR_\alpha = 1$ if and only if $QSR_\alpha(S, T) = QSR_\alpha(\overline{S}, \overline{T}) = QSR_\alpha(S, \overline{T}) = QSR_\alpha(\overline{S}, T) = 1$.

b) For $\alpha = k$, $QSR_\alpha = 1$.

The interpretation of $QSR_\alpha(E, F) = \pm 1$ is that in the quadrant $E \times F$ the residuals have one sign; and this is a signal for very influential cells or columns or rows. Example 1 explains this fact. So Lemma 2 provides a necessary and sufficient condition for $QSR_\alpha = 1$, which is not true for $\tau_1(\alpha)$ and $\tau_2(\alpha)$. Geometry plays its unique role.

Notation: $QSR_\alpha(+) = \{QSR_\alpha(S, T), QSR_\alpha(\overline{S}, \overline{T})\}$ and $QSR_\alpha(-) = \{QSR_\alpha(S, \overline{T}), QSR_\alpha(\overline{S}, T)\}$.

Remark: The computation of the elements of $QSR_\alpha(\cdot)$ and $QSR_\alpha(\cdot)$ are done easily in the following way. We note that the $\alpha$th principal axis can be written as $u_\alpha = u_\alpha + u_\alpha -$, where $u_\alpha + = (u_\alpha + 1_I)/2$ and $u_\alpha - = (u_\alpha - 1_I)/2$; similarly $v_\alpha = v_\alpha + v_\alpha -$.

Remark: The computation of the elements of $QSR_\alpha(\cdot)$ and $QSR_\alpha(\cdot)$ are done easily in the following way. We note that the $\alpha$th principal axis can be written as $u_\alpha = u_\alpha + u_\alpha -$, where $u_\alpha + = (u_\alpha + 1_I)/2$ and $u_\alpha - = (u_\alpha - 1_I)/2$; similarly $v_\alpha = v_\alpha + v_\alpha -$, where $v_\alpha + = (v_\alpha + 1_I)/2$ and $v_\alpha - = (v_\alpha - 1_I)/2$, where $1_I$ designates a column vector of 1’s of size $I$. So

\[
QSR_\alpha(S, T) = \frac{\delta_\alpha/4}{v_\alpha + abs(X_\alpha)u_\alpha +},
\]

\[
QSR_\alpha(\overline{S}, \overline{T}) = \frac{\delta_\alpha/4}{v_\alpha - abs(X_\alpha)u_\alpha -},
\]

\[
QSR_\alpha(S, \overline{T}) = \frac{\delta_\alpha/4}{v_\alpha + abs(X_\alpha)u_\alpha +},
\]

\[
QSR_\alpha(\overline{S}, T) = \frac{\delta_\alpha/4}{v_\alpha - abs(X_\alpha)u_\alpha -},
\]

where $abs(X_\alpha) = (|X_\alpha(i, j)|)$.

5 Examples

Here we present the analysis of two contingency tables and one compositional data set.
5.1 Xlstat demoCA count data set

Table 1 is a small data set of size $7 \times 4$, as the title suggests to introduce CA in the software Xlstat available by a google search on the web.

Table 1: Xlstat demoCA count table.

| Attribute | Age  | Bad | Average | Good | VeryGood |
|-----------|------|-----|---------|------|----------|
| 16-24     | 69   | 49  | 48      | 41   |
| 25-34     | 148  | 45  | 14      | 22   |
| 35-44     | 170  | 65  | 12      | 29   |
| 45-54     | 159  | 57  | 12      | 28   |
| 55-64     | 122  | 26  | 6       | 18   |
| 65-74     | 106  | 21  | 5       | 23   |
| 75+       | 40   | 7   | 1       | 14   |

Table 2: $10^3 \times$ Xlstat demoCA count table TCA centered.

| Attribute | Age  | Bad       | Average | Good    | VeryGood | row sum |
|-----------|------|-----------|---------|---------|----------|---------|
| 16-24(a)  | 69   | -40.66    | 5.76    | 24.36   | 10.54    | 0       |
| 25-34(b)  | 148  | 7.84      | -0.42   | -1.87   | -5.55    | 0       |
| 35-44(c)  | 170  | 3.27      | 7.43    | -5.85   | -4.86    | 0       |
| 45-54(d)  | 159  | 4.00      | 4.47    | -4.78   | -3.69    | 0       |
| 55-64(e)  | 122  | 13.87     | -6.06   | -4.73   | -3.08    | 0       |
| 65-74(f)  | 106  | 9.60      | -7.25   | -4.56   | 2.22     | 0       |
| 75+(g)    | 40   | 2.07      | -3.93   | -2.56   | 4.42     | 0       |

column sum | 0     | 0         | 0       | 0       | 0        | 0       |
Table 3: $10^3$×Xlstat demoCA count table TLRA centered.

| Age   | Attribute |  |  |  |  |  |
|-------|-----------|---|---|---|---|---|
|       | Bad       | VeryGood | Good | Average | row sum |
| 16-24 | -0.9994  | -0.0309  | 1.1679  | -0.1377  | 0  |
| 25-34 | 0.0579    | -0.3592  | 0.2299  | 0.0714   | 0  |
| 35-44 | 0.0394    | -0.2401  | -0.0813 | 0.2820   | 0  |
| 45-54 | 0.0308    | -0.2168  | -0.0230 | 0.2090   | 0  |
| 55-64 | 0.3122    | -0.1124  | -0.1699 | -0.0298  | 0  |
| 65-74 | 0.2444    | 0.2055   | -0.2794 | -0.1705  | 0  |
| 75+   | 0.3146    | 0.7538   | -0.8441 | -0.2244  | 0  |
| col sum | 0       | 0        | 0      | 0        | 0  |

Tables 2 and 3 display two different ways of double centering the data in TCA and LRA. It is evident that corresponding residuals in both entries can be different, thus producing probably different quality maps, even though we shall use the same algorithm in the sequel.

Let us describe in a nutshell what TSVD does on the TCA residuals in Table 2. Our aim is to partition the TCA residuals into four quadrants by permuting the rows and the columns in such a way that the signs in each quadrant are mostly constant; or equivalently by maximizing $QSR_1$ index. The number of nontrivial partitions is: $(2^I - 2)(2^J - 2)$. For TCA, the partition that maximizes $QSR_1 = 81.43\%$ is delineated in Table 2, where: $S = \{VeryGood, Good, Average\}$ and $\overline{S} = \{Bad\}$, and, $T = \{a\}$ and $\overline{T} = \{b, c, d, e, f, g\}$. Note that

$$QSR_1(+) = \{QSR_1(S, T) = 100, QSR_1(\overline{S}, \overline{T}) = 100\}$$

as reported in Table 4: because the residuals in the quadrant $S \times T$ are all positive $\{5.76, 24.36, 10.54\}$, and, the residuals in the quadrant $\overline{S} \times \overline{T}$ are all positive $\{7.84, 3.27, 4, 13.87, 9.6, 2.07\}$. Similarly as reported in Table 4,

$$QSR_1(-) = \{QSR_1(S, \overline{T}) = -52.29, QSR_1(\overline{S}, T) = -100\}.$$

$QSR_1(S, \overline{T}) = -52.29$ is quite low, because the quadrant $S \times \overline{T}$ has 18 residuals of which four have positive sign and 14 negative sign; while $QSR_1(\overline{S}, T) =$
−100, because the quadrant $S \times T$ is a singleton \{−40.66\}; so the singleton cell produces one heavyweight column, “bad” and one heavyweight row, “16-24”, but it is not a heavyweight cell, because its weight does not go to infinity as discussed in Choulakian (2008). Furthermore, we also note that the first taxicab dispersion $\delta_1 = 4 \frac{|-40.66|}{1000} = 0.1626$, because of (16). The column $Bad$ and the age group 16 − 24 dominate the first dimension of the TCA map in Figure 1.

Note that the optimal partitions in Table 2 and Table 3 are different.

Figure 1 displays both TCA and TLRA maps of the data with distinct colors for age category and modality. We note the following two facts. First, the TCA and TLRA maps are quite different; second, the TLRA map in Figure 1 is much more interpretable than the corresponding TCA map, because the age groups are ordered on the first axis in the TLRA map.

Table 4 displays the intrinsic measures of quality of the signs of the residuals, QSR values, for the first two principal dimensions for TCA and TLRA. TLRA values are $QSR_1 = 87.69$ and $QSR_2 = 94.90$, which are higher than the corresponding TCA values $QSR_1 = 81.43$ and $QSR_2 = 86.79$. So the QSR values confirm what we saw visually.

Table 4: QSR (%) of Xlstat demoCA data.

| $\alpha$ | $QSR_\alpha$ (+) | $QSR_\alpha$ (−) | $QSR_\alpha$ | $\delta_\alpha$ |
|----------|------------------|------------------|-------------|-------------|
| 1        | (100, 100)       | (−100, −52.29, ) | 81.43       | 0.1626      |
| 2        | (100, 83.74)     | (−100, −70.69)   | 86.79       | 0.0545      |

| $\alpha$ | $QSR_\alpha$ (+) | $QSR_\alpha$ (−) | $QSR_\alpha$ | $\delta_\alpha$ |
|----------|------------------|------------------|-------------|-------------|
| 1        | (78.02, 88.43)   | (−100, −87.02)   | 87.69       | 6.8725      |
| 2        | (90.76, 99.44)   | (−99.44, −90.76) | 94.90       | 4.390       |

The last column in Table 4 displays the first two taxicab dispersion values $\delta_\alpha$ for $\alpha = 1, 2$ for the two methods, which are not comparable.

5.2 English authors count data

This is a sparse contingency table cross-classifying known english authors according to their geographical origins described by 50 counties and 12 periods of length 25 years extending from 1300-1600; it can be found in Genet (2002). For TLRA computations we have added 1 to all counts, a procedure suggested by Tukey (1977, p. 257), which keeps the re-expressed log-counts
Table 1: Maps of DemoCA data.
nonnegative. Figure 2 displays the TCA and TLRA maps of the data. It is showing only the 12 periods. We note the following facts: The TCA map is more interpretable than the TLRA map. We interpret the TCA map in the following way: by grouping the first seven periods extending from 1300 to 1475, we obtain a parabolic structure on the principal plane which shows the evolution of the geographical origins of the authors described by the countries. For further details concerning TCA of sparse contingency tables, refer to Choulakian (2017).

Table 5 presents the QSR values for the first four principal dimensions: We choose the TCA method because its $QSR_1 = 54.81$ and $QSR_2 = 50.29$ indices are higher by 10% than the corresponding TLRA values $QSR_1 = 43.28$ and $QSR_2 = 40.97$.

Table 5: QSR (%) of Authors data for the first 4 dimensions.

| α  | $QSR_α(−)$ | $QSR_α(+)$ | $QSR_α$ | $δ_α$ |
|----|------------|------------|---------|-------|
| 1  | (-84.19, -44.35) | (73.56, 40.06) | 54.81   | 0.2380 |
| 2  | (-67.31, -44.15) | (67.84, 36.64) | 50.29   | 0.1975 |
| 3  | (-49.54, -57.58) | (43.18, 60.27) | 51.74   | 0.1753 |
| 4  | (-44.84, -59.85) | (42.21, 50.78) | 48.5    | 0.1373 |

| α  | $QSR_α(−)$ | $QSR_α(+)$ | $QSR_α$ | $δ_α$ |
|----|------------|------------|---------|-------|
| 1  | (-48.87, -38.53) | (50.56, 38.14) | 43.28   | 93.6699 |
| 2  | (-33.02, -47.97) | (40.99, 45.24) | 40.97   | 78.2741 |
| 3  | (-45.79, -46.63) | (31.30, 59.29) | 43.43   | 74.8385 |
| 4  | (-38.67, -51.99) | (55.55, 33.78) | 43.15   | 66.8444 |

5.3 Food compositional data

The food compositional data set is of size 25 by 9 and analyzed quite in detail by CODA-LRA in Pawlowsky-Glahn and Egozcue (2011). These data are percentages of consumption of 9 different kinds of food in 25 countries in Europe in the early eighties. The 9 different kinds of food are: red meat (RM); white meat (WM); fish (F); eggs (E); milk (M); cereals (C); starch (S); nuts (N); fruit and vegetables (FV). The 25 countries are divided into 16 western (w) and 9 eastern (e) countries. It is evident that in Table 6, TCA $QSR_1 = 77.89$ value is significantly higher than the TLRA $QSR_1 = 68.69$, so we choose TCA over TLRA. In Figure 3 are displayed the TCA and TLRA.
Table 2: Maps of Authors data.
maps where the 9 food kinds are represented by their symbols and the 25
countries by their symbols eastern (e) or western (w). The TCA map dis-
criminates much better the eastern and the western countries than the TLRA
map: All eastern countries (except 1 located in the first quadrant) are clus-
tered in the third quadrant. We also note that TLRA map is very similar to
LRA map in Pawlowsky-Glahn and Egozcue (2011).

Table 6: QSR (%) of Food data for the first 4 dimensions.

| α  | QSR_α(+) | QSR_α(-) | QSR_α | δ_α  |
|----|---------|---------|-------|------|
| 1  | 86.58, 71.16 | -96.04, -65.21 | 77.89 | 0.2524 |
| 2  | 56.01, 61.84  | -64.99, -46.48  | 56.40 | 0.1041 |
| 3  | 83.11, 41.49  | -68.57, -54.06  | 57.79 | 0.0848 |
| 4  | 65.59, 64.28  | -69.82, -54.48  | 63.01 | 0.0701 |

| TLRA |
|------|
| α  | QSR_α(+) | QSR_α(-) | QSR_α | δ_α  |
| 1  | 87.43, 63.19 | -89.99, -50.36 | 68.69 | 61.9773 |
| 2  | 47.57, 68.06  | -62.51, -47.07  | 54.83 | 34.6618 |
| 3  | 71.49, 61.51  | -62.47, -62.94  | 64.37 | 32.4594 |
| 4  | 60.55, 51.41  | -61.03, -52.59  | 56.05 | 20.4148 |

6 Minimal R script

We show a minimal R script that can be executed to obtain the results in
this paper. A more extensive script will be available in the CRAN repository.

We follow the three steps procedure outlined in section 3. We suppose
that the data is in a matrix form.

- Step 1 (centering): different for each method.
- Step 2 (computation of contribution scores and QSR index): common
to both TCA and TLRA methods. This step calls the function TSVD.r
from the R Package TaxicabCA.
- Step 3 (visualisation). It uses the plot function from TaxicabCA. For
  TCA, it suffices to use the TaxicabCA plot function. For TRLA, we
Table 3: Maps of Food compositional data.
must create a partial tca object in order to use the TaxicabCA plot function.

### Step 0: Preliminaries

# Install the 2 packages and the center_scale function

- a. library(TaxicabCA)
- b. library(GA)
- c. center_scale <- function(x) { scale(x, scale = FALSE) }

# dataMatrix holds the raw data

# 7x4 dataMatrix of Example 1
dataMatrix <- matrix(c(69,49,48,41,
148,45,14,22,
170,65,12,29,
159,57,12,28,
122,26,6,18,
106,21,5,23,
40,7,1,14),nrow=7,ncol=4,byrow=T)
rownames(dataMatrix) <- c("16-24", "25-34",
"35-44", "45-54", "55-64", "65-74", "75+")
colnames(dataMatrix) <- c("Bad", "Average", "Good", "VeryGood")
# rownames and colnames are used to label points
dataName <- "XLStatCAData" # Will appear in the figure title

# Uncomment ONE of the following lines
# to choose the centering method
# centeringMethod <- "TCA"
centeringMethod <- "TLRA"
# ncol(centeredDataMatrix))
# For this illustration, must have nAxes ≥ 2
nAxes <- 2
dataMatrix <- as.matrix(dataMatrix)

### Step 1: Centering the data matrix:
# According to the centering method chosen ABOVE

if (centeringMethod == "TCA") {
    Proba <- dataMatrix/sum(dataMatrix)
    rowProba <- apply(Proba,1,sum)
    colProba <- apply(Proba,2,sum)
    centeredDataMatrix <- Proba - rowProba %*% t(colProba)
}

# TLRA Centering
if (centeringMethod == "TLRA") {
    centeredDataMatrix <- log(dataMatrix)
    centeredDataMatrix <- scale(centeredDataMatrix, scale = FALSE)
    centeredDataMatrix <- t(scale(t(centeredDataMatrix), scale = FALSE))
    attr(centeredDataMatrix, "scaled:center") <- NULL
}

library(TaxicabCA)

### Step 2: Compute the Taxicab SVD for the centered matrix

# Common to both methods
nRow <- nrow(centeredDataMatrix)
ncol <- ncol(centeredDataMatrix)
axesNames <- paste("Axis", 1:nAxes, sep="")

# Create the matrices required to receive the results
rowScores <- matrix(NA, nrow = nRow, ncol = nAxes)
rownames(rowScores) <- rownames(centeredDataMatrix)
colScores <- matrix(NA, ncol = nCol, nrow = nAxes)
colnames(colScores) <- colnames(centeredDataMatrix)
dispersion <- rep(NA, nAxes) # matrix(0, nrow = nAxes, ncol = 1)
QSR <- matrix(NA, nrow = nAxes, ncol = 5)
colnames(QSR) <- c("VUQuadrant1", "VUQuadrant3", "VUQuadrant2", "VUQuadrant4", "All")
rownames(QSR) <- colnames(rowScores) <- rownames(colScores) <- names(dispersion)
residuals <- centeredDataMatrix

iiAxis <- 1
for (iiAxis in 1:nAxes) {
    # The search functions come from TaxicabCA
# Uncomment ONE search method - As of 2020, on a desktop computer,
# Exhaustive is only feasible for nRow < 22
axisResult <- SearchExhaustive(residuals)
axisResult <- SearchCrissCross(residuals)
axisResult <- SearchGeneticAlgorithm(residuals)
# Note: Some versions of TaxicaCA misspell “Algorithm”!
U <- axisResult$uMax
dispersion[iiAxis] <- axisResult$L1Max
rowScores[, iiAxis] <- residuals %*% t(axisResult$uMax)
V <- sign(rowScores[, iiAxis, drop = F])
colScores[iiAxis, ] <- t(V) %*% residuals
# Compute the quality of the signs of
# the residuals (QSR) for each UV “quadrant”
QSR[iiAxis,1] <- 0.25/sum(abs(residuals[V > 0, U > 0]))
QSR[iiAxis,2] <- 0.25/sum(abs(residuals[V < 0, U < 0]))
QSR[iiAxis,4] <- -0.25/sum(abs(residuals[V > 0, U < 0]))
QSR[iiAxis,3] <- -0.25/sum(abs(residuals[V < 0, U > 0]))
# Compute the overall quality of the signs of the residuals
# abs(QSR[iiAxis,1:4])/(1/sum(abs(residuals)))
QSR[iiAxis,5] <- 1/sum(abs(residuals))
QSR[iiAxis,] <- dispersion[iiAxis]*QSR[iiAxis,]
# Update the residuals for the next iteration
residuals <- residuals - (rowScores[, iiAxis, drop = F] %*% colScores[iiAxis,drop = F])/dispersion[iiAxis]
}

### Step 3: Visualisation
# TCA Visualisation
if (centeringMethod == “TCA”) {
# tca can choose a search method automatically
Data.tca <- tca(dataMatrix, nAxes=nAxes)
Data.tca$dataName <- paste(dataName,”TCA”,sep = “ - ”)
# Open a graphics window outside of RStudio (if RStudio is used)
dev.new(noRStudioGD = TRUE)
# Call plot.tca from TaxicabCA (Data.tca is class “tca”)
plot(Data.tca,labels.rc = c(1, 1),cex.rc = c(.8,.8))
}
# TLRA Visualisation
if (centeringMethod == "TLRA") {
  rowScores <- nRow*rowScores
  colScores <- nCol*colScores
  Data.tlra <- list(rowScores = rowScores, colScores = colScores,
                    dispersion = dispersion,
                    dataName = paste(dataName, "TRLA", sep = " - ")
  )
  # Add class "tca" to the class of the list in order to
  # call plot.tca from TaxicabCA automatically
  class(Data.tlra) <- c(class(Data.tlra), "tca")
  # Open a graphics window outside of RStudio (if RStudio is used)
  dev.new(noRStudioGD = TRUE)
  # Call plot.tca from TaxicabCA - Data.tlra is class "tca"
  # Use labels.rc = c(1,1) only if the data has rown and colnames.
  # Otherwise, use labels.rc = c(0,0), c(1,0) or c(0,1)
  plot(Data.tlra, labels.rc = c(1,1), cex.rc = c(.8, .8))
}

# Print the numerical results
print(dataName)
print(centeringMethod)
print(dispersion)
print(QSR)

7 Conclusion

We attained two aims in this paper. First, we introduced the package Taxi-
cabCA in R and showed its functionalities. Second, we applied it to study the
influence of two different centering procedures in two well developed meth-
ods CA and LRA. In both aims, the tool was TSVD, which has some nice
mathematical properties.

In this paper we only considered unweighted LRA analysis as developed
in Goodman (1991, equation 2.2.1) or Aitchison (1986). We did not tackle
weighted LRA analysis as discussed in Goodman (1991, equation 2.2.7) and
Greenacre and Lewi (2009), because the weighted residual matrix is not
uniformly centered, so TSVD will produce biased results because equations
(15,16) will not be satisfied.
There are two perspectives for data analysis of contingency tables or compositional data. The first, based on the mathematical fact that the rows or the columns are found on the probability simplex, is CA/LRA based on invariance principles: such as principle of distributional equivalence, and, the principle of scale invariance and the principle of subcompositional coherence. The second is on re-expression and the analysis of residuals advocated by Tukey (1977, in particular chapters 10 and 15). This paper develops jointly the use of both perspectives by introducing the use of QSR index describing the concentration of the sign of the residuals in re-expressed count or compositional data, and thus choosing the method. We think our novel approach will especially be fruitful for large data sets, such as microbiome data.

We conclude by citing Tukey (1977, p.400): "the general maxim—it is a rare thing that a specific body of data tells us clearly enough how it itself should be analyzed—applies to choice of re-expression for two-way analysis". For contingency tables and compositional data, the choice of re-expression is essentially between equations (11) and (14).

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