Title
Distance-Based Transformations of Biplots

Author
Jan de Leeuw

Publication Date
2011-10-25

DISTANCE-BASED TRANSFORMATIONS OF BIPLOTS

JAN DE LEEUW

1. Introduction

In principal component analysis and related techniques we approximate (in the least squares sense) an $n \times m$ matrix F by an $n \times m$ matrix G which satisfies $\mathbf{rank}(G) \leq p$, where $p < \min(n, m)$. Or, equivalenty, we want to find an $n \times p$ matrix X and an $m \times p$ matrix Y such that $G = XY'$ approximates F as closely as possible. The rows of X and Y are then often used in graphical displays. In particular, *biplots* [Gower and Hand, 1996] represent X and Y jointly as $n + m$ points in Euclidean p space.

If formulated in this way, there is an important form of indeterminacy in this approximation problem. If R of order p is nonsinsular, then we can define $\tilde{X} = XR$ and $\tilde{Y} = YR^{-T}$ and we have $\tilde{X}\tilde{Y}' = XY'$, where A^{-T} is the transpose of the inverse (or the inverse of the transpose). Thus $\tilde{X}$ and $\tilde{Y}$ give exactly the same approximation, but plotting them may give quite different results, depending on R. To give a simple example, we can choose R scalar, and make $\tilde{X}$ arbitrarily small and $\tilde{Y}$ arbitrarily big. In particular for biplots, which are often interpreted in terms of distances between the points, the indeterminacy is a nuisance and can lead to unattractive representations.

In this note we choose R in such a way that the distances, more specifically the squared Euclidean distances, between selected rows of $\tilde{X}$ and $\tilde{Y}$ are small. This takes care of both the relative scaling of the two clouds of points, as well as rotating them to some form of conformance.

Date: April 14, 2006.

2000 *Mathematics Subject Classification.* 62H25.

Key words and phrases. Multivariate Analysis.

2. Problem Formulation

The squared distance between rows i and j of the $n + m$ matrix

$$Z = \begin{bmatrix} XR \\ YR^{-T} \end{bmatrix}$$

can be written as

$$d_{ij}^2(R) = (e_i - e_j)'C(e_i - e_j) = \mathbf{tr}\ CA_{ij}.$$

Here the e_i are unit vectors (columns of the identity matrix) and we define

$$C = \begin{bmatrix} XSX' & XY' \\ YX' & YS^{-1}Y' \end{bmatrix},$$

as well as $S = RR'$ and $A_{ij} = (e_i - e_j)(e_i - e_j)'$.

Thus summing over a selected subset $\mathcal{I}$ of squared distances leads to a loss function of the form

$$\lambda(S) = \sum_{(i,j)\in\mathcal{I}} d_{ij}^2(S) = \mathbf{tr}\ SX'A_{11}X + \mathbf{tr}\ S^{-1}Y'A_{22}Y$$

where A_{11} and A_{22} are the two principal submatrices of

$$A = \sum_{(i,j)\in\mathcal{I}} A_{ij}.$$

If we minimize the sum of squares of all nm distances between the n points in X and the m points in Y, for example, we find $A_{11} = mI$ and $A_{22} = nI$. If $n = m$ and we want to minimize the sum of the n squared distances between the corresponding points x_i and y_i then $A_{11} = A_{22} = I$.

3. Problem Solution

Let us minimize $\lambda(S) = \mathbf{tr}\ SP + \mathbf{tr}\ S^{-1}Q$, where both P and Q are positive definite. If P and/or Q are singular, the more general results of De Leeuw [1982] must be used, but in most applications we have in mind non-singularity is guaranteed.

The stationary equations for the problem of minimizing $\lambda(S)$ are

$$P = S^{-1}QS^{-1}, \tag{1}$$

which we have to solve for a positive definite S. We can use the symmetric square root to rewrite Equation (1) as

$$I = P^{-\frac{1}{2}}S^{-1}P^{-\frac{1}{2}}\left[P^{\frac{1}{2}}QP^{\frac{1}{2}}\right]P^{-\frac{1}{2}}S^{-1}P^{-\frac{1}{2}}, \tag{2}$$

from which

$$P^{-\frac{1}{2}}S^{-1}P^{-\frac{1}{2}} = \left[P^{\frac{1}{2}}QP^{\frac{1}{2}}\right]^{-\frac{1}{2}}, \tag{3}$$

and thus

$$S^{-1} = P^{\frac{1}{2}}\left[P^{\frac{1}{2}}QP^{\frac{1}{2}}\right]^{-\frac{1}{2}}P^{\frac{1}{2}}, \tag{4}$$

and

$$S = P^{-\frac{1}{2}}\left[P^{\frac{1}{2}}QP^{\frac{1}{2}}\right]^{\frac{1}{2}}P^{-\frac{1}{2}}. \tag{5}$$

If we want to minimize the sum of squares of all distances between the points in X and those in Y we have seen that $A_{11} = mI$ and $A_{22} = nI$. In many forms of principal component analysis X is chosen such that $X'X = I$, and thus $P = mI$. In that case, from (5),

$$S = \sqrt{\frac{n}{m}}(Y'Y)^{\frac{1}{2}}.$$

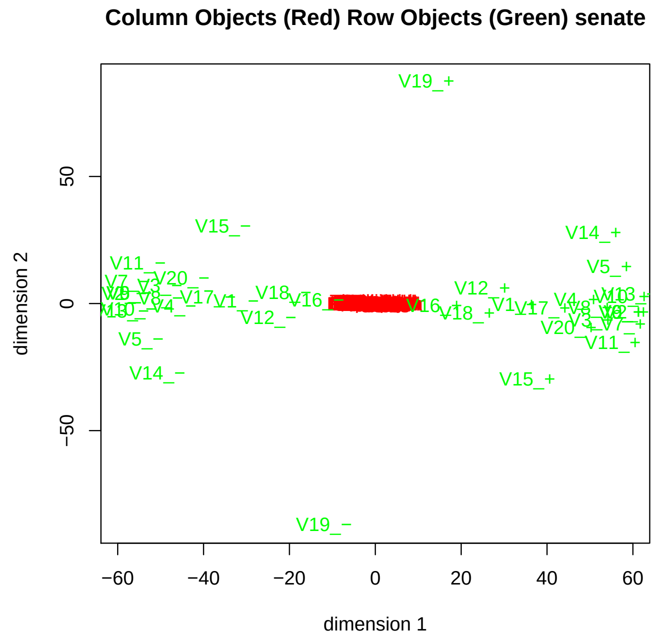
If $Y = L\Lambda L'$ is an eigen-decomposition of Y, we can choose

$$R = \left[\frac{n}{m}\right]^{\frac{1}{4}} L\Lambda^{\frac{1}{4}},$$

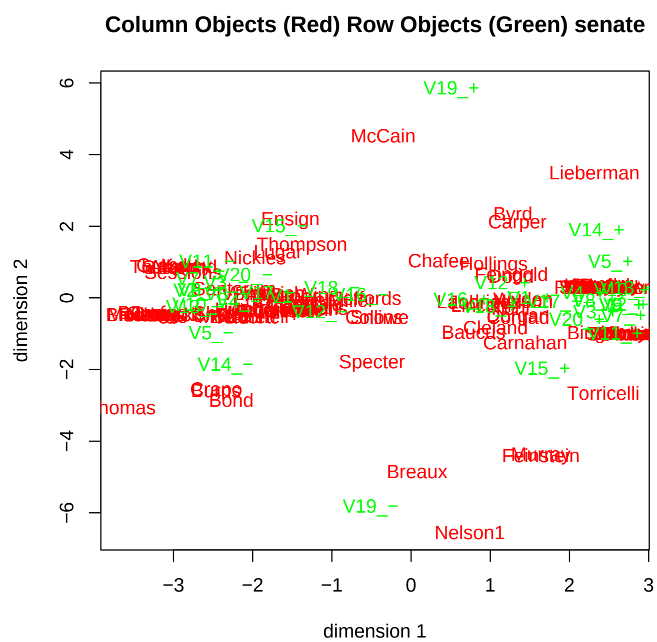
$$R^{-T} = \left[\frac{m}{n}\right]^{\frac{1}{4}} L\Lambda^{-\frac{1}{4}}.$$

4. Example

To illustrate the problem, consider the following output from the scalAssoc() program [De Leeuw, 2006]. These are 20 votes of 100 US senators. Each vote is presented by a plus ("aye") point and a minus ("nay") point, and the technique jointly scales senators and votes in such a way that senators are closest to the vote points they endorse. Or, equivalently, senators voting “aye” must be separated by a straight line from senators voting “nay”. In Figure 1 all senators are clumped around the origin, and this makes it impossible to read and interpret the plot.



Now let us apply the scaling outlines in this paper. Figure 2 gives the results, which are clearly much more satisfactory.



References

J. De Leeuw. Majorization Methods for Distance Association Models. Technical report, UCLA Department of Statistics, 2006.

J. De Leeuw. Generalized Eigenvalue Problems with Positive Semidefinite Matrices. *Psychometrika*, 47:87–94, 1982.

J.C. Gower and D.J. Hand. *Biplots*. Number 54 in Monographs on Statistics and Applied Probability. Chapman and Hall, 1996.

Department of Statistics, University of California, Los Angeles, CA 90095-1554

E-mail address, Jan de Leeuw: `deleeuw@stat.ucla.edu`

URL, Jan de Leeuw: `http://gifi.stat.ucla.edu`