DISTANCE-BASED TRANSFORMATIONS OF BIPLOTS

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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.

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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 nonsingularity 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),

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

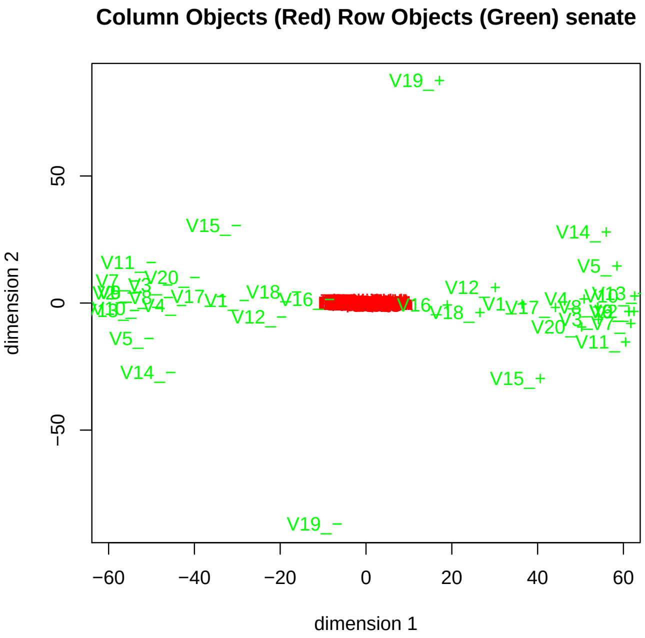
If $Y = L\Lambda L'$ is an eigen-decomposition of Y, we can choose

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

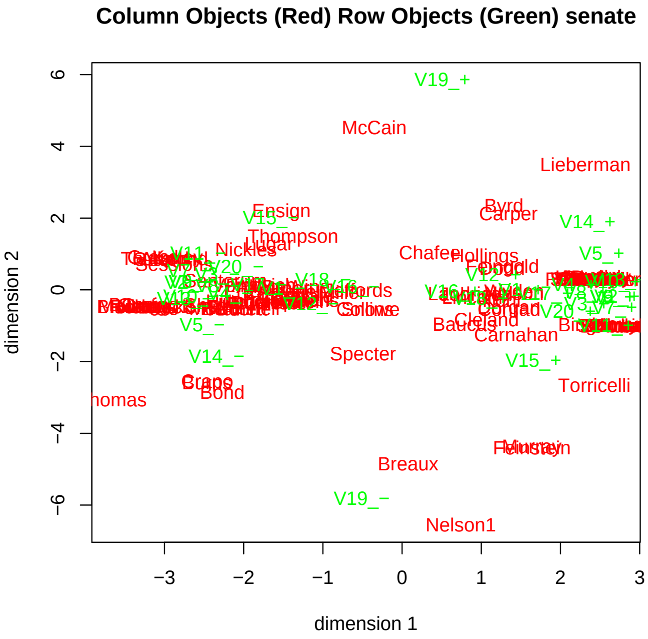
$$R^{-T} = \left[\frac{m}{n}\right]^{\frac{1}{4}} L\Lambda^{-\frac{1}{4}}.$$

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.



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