HOMALS

The iterative HOMALS algorithm is a modernized version of Guttman (1941). The treatment of missing values, described below, is based on setting weights in the loss function equal to zero, and was first described in De Leeuw and Van Rijckevorsel (1980). Other possibilities do exist and can be accomplished by recoding the data (Gifi, 1981; Meulman, 1982).

Notation

The following notation is used throughout this chapter unless otherwise stated:

n	Number of cases (objects)
m	Number of variables
p	Number of dimensions

For variable j, $j = 1, \ldots, m$

$\mathbf{h}_j$	n-vector with categorical observations
k_j	Number of valid categories (distinct values) of variable j
$\mathbf{G}_j$	Indicator matrix for variable j, of order $n \times k_j$

$$g_{(j)ir} = \begin{cases} 1 & \text{when the } i\text{th object is in the } r\text{th category of variable } j \\ 0 & \text{when the } i\text{th object is not in the } r\text{th category of variable } j \end{cases}$$

$\mathbf{M}_j$	Binary, diagonal $n \times n$ matrix, with diagonal elements defined as

$$m_{(j)ii} = \begin{cases} 1 & \text{when the } i\text{th observation is within the range } [1, k_j] \\ 0 & \text{when the } i\text{th observation is outside the range } [1, k_j] \end{cases}$$

$\mathbf{D}_j$	Diagonal matrix containing the univariate marginals, i.e., the column sums of G_j.

The quantification matrices are

X	Object scores, of order $n \times p$
$\mathbf{Y}_j$	Category quantifications, of order $k_j \times p$
Y	Concatenated category quantification matrices, of order $\sum_j k_j \times p$.

Note: The matrices $\mathbf{G}_j$, $\mathbf{M}_j$, and $\mathbf{D}_j$ are exclusively notational devices; they are stored in reduced form, and the program fully profits from their sparseness by replacing matrix multiplications with selective accumulation.

Objective Function Optimization

The HOMALS objective is to find object scores **X** and a set of $\mathbf{Y}_j$ (for $j = 1, \ldots, m$) so that the function

$$\sigma(\mathbf{X}; \mathbf{Y}) = 1/m \sum_j \mathrm{tr}\left(\left(\mathbf{X} - \mathbf{G}_j \mathbf{Y}_j\right)' \mathbf{M}_j \left(\mathbf{X} - \mathbf{G}_j \mathbf{Y}_j\right) \right)$$

is minimal, under the normalization restriction $\mathbf{X}' \mathbf{M}_* \mathbf{X} = mn\mathbf{I}$, where the matrix $\mathbf{M}_* = \sum_j \mathbf{M}_j$, and **I** is the $p \times p$ identity matrix. The inclusion of $\mathbf{M}_j$ in $\sigma(\mathbf{X}; \mathbf{Y})$ ensures that there is no influence of data values outside the range $[1, k_j]$, which may be really missing or merely regarded as such; $\mathbf{M}_*$ contains the number of "active" data values for each object. The object scores are also centered; that is, they satisfy $\mathbf{u}' \mathbf{M}_* \mathbf{X} = 0$, with **u** denoting an n-vector with ones.

Optimization is achieved through the following iteration scheme:
1. Initialization
2. Update object scores
3. Orthonormalization
4. Update category quantifications
5. Convergence test: repeat steps 2-4 or continue
6. Rotation

These steps are explained below.

1. **Initialization**

   The object scores $\mathbf{X}$ are initialized with random numbers, which are normalized so that $\mathbf{u}'\mathbf{M}_*\mathbf{X} = 0$ and $\mathbf{X}'\mathbf{M}_*\mathbf{X} = mn\mathbf{I}$, yielding $\tilde{\mathbf{X}}$. Then the first category quantifications are obtained as $\tilde{\mathbf{Y}}_j = \mathbf{D}_j^{-1}\mathbf{G}_j'\tilde{\mathbf{X}}$.

2. **Update object scores**

   First the auxiliary score matrix $\mathbf{Z}$ is computed as

   $$\mathbf{Z} \leftarrow \sum_j \mathbf{M}_j\mathbf{G}_j\tilde{\mathbf{Y}}_j$$

   and centered with respect to $\mathbf{M}_*$:

   $$\tilde{\mathbf{Z}} \leftarrow \left\{\mathbf{M}_* - \left(\mathbf{M}_*\mathbf{u}\mathbf{u}'\mathbf{M}_*/\mathbf{u}'\mathbf{M}_*\mathbf{u}\right)\right\}\mathbf{Z}.$$

   These two steps yield locally the best updates when there are no orthogonality constraints.

3. **Orthonormalization**

   The orthonormalization problem is to find an $\mathbf{M}_*$-orthonormal $\mathbf{X}^+$ that is closest to $\tilde{\mathbf{Z}}$ in the least squares sense. In HOMALS, this is done by setting

   $$\mathbf{X}^+ \leftarrow m^{1/2}\mathbf{M}_*^{-1/2}\,\mathrm{GRAM}\left(\mathbf{M}_*^{-1/2}\tilde{\mathbf{Z}}\right)$$

   which is equal to the genuine least squares estimate up to a rotation. The notation GRAM( ) is used to denote the Gram-Schmidt transformation (Björk and Golub, 1973).

4. **Update category quantifications**

   For $j = 1, \ldots, m$ the new category quantifications are computed as:

   $$\mathbf{Y}_j^+ = \mathbf{D}_j^{-1}\mathbf{G}_j'\tilde{\mathbf{X}}$$

5. **Convergence test**

   The difference between consecutive loss function values $\sigma(\tilde{\mathbf{X}};\tilde{\mathbf{Y}}) - \sigma(\mathbf{X}^+;\mathbf{Y}^+)$ is compared with the user-specified convergence criterion ε —a small positive number. Steps 2 to 4 are repeated as long as the loss difference exceeds ε.

6. **Rotation**

   As indicated in step 3, during iteration the orientation of $\mathbf{X}$ and $\mathbf{Y}$ with respect to the coordinate system is not necessarily correct; this also reflects that $\sigma(\mathbf{X};\mathbf{Y})$ is invariant under simultaneous rotations of $\mathbf{X}$ and $\mathbf{Y}$. From theory it is known that solutions in different dimensionality should be nested; that is, the p-dimensional solution should be equal to the first p columns of the $(p+1)$-dimensional solution. Nestedness is achieved by computing the eigenvectors of the matrix $1/m \sum_{j} \mathbf{Y}_j'\mathbf{D}_j\mathbf{Y}_j$. The corresponding eigenvalues are printed after the convergence message of the program. The calculation involves tridiagonalization with Householder transformations followed by the implicit QL algorithm (Wilkinson, 1965).

Diagnostics

Maximum Rank (may be issued as a warning when exceeded)

The maximum rank $p_{\max}$ indicates the maximum number of dimensions that can be computed for any data set. In general we have:

$$p_{\max} = \min\left\{(n-1), \left(\left(\sum_{j} k_j\right) - \max(m_1, 1)\right)\right\},$$

where m_1 is the number of variables with no missing values. Although the number of nontrivial dimensions may be less than $p_{\max}$ when $m = 2$, HOMALS does allow dimensionalities all the way up to $p_{\max}$.

Marginal Frequencies

The frequencies table gives the univariate marginals and the number of missing values (that is, values that are regarded as out of range for the current analysis) for each variable. These are computed as the column sums of $\mathbf{D}_j$ and the total sum of $\mathbf{M}_j$.

Discrimination Measure

These are the dimensionwise variances of the quantified variables. For variable j and dimension s, we have

$$\eta_{js}^2 = \mathbf{y}'_{(j)s}\mathbf{D}_j\mathbf{y}_{(j)s}\big/n\,,$$

where $\mathbf{y}_{(j)s}$ is the sth column of $\mathbf{Y}_j$, corresponding to the sth quantified variable $\mathbf{G}_j\mathbf{y}_{(j)s}$.

Eigenvalues

The computation of the eigenvalues that are reported after convergence is discussed in step 6. With the HISTORY option, the sum of the eigenvalues is reported during iteration under the heading "total fit." Due to the fact that the sum of the eigenvalues is equal to the trace of the original matrix, the sum can be computed as $1/m\sum_j\sum_s\eta_{js}^2$. The value of $\sigma(\mathbf{X};\mathbf{Y})$ is equal to $p-1/m\sum_j\sum_s\eta_{js}^2$.

References

Björk, A., and Golub, G. H. 1973. Numerical methods for computing angles between linear subspaces. *Mathematics of Computation*, 27: 579–594.

De Leeuw, J., and Van Rijckevorsel, J. 1980. HOMALS and PRINCALS—Some generalizations of principal components analysis. In: *Data Analysis and Informatics*, E. Diday et al, eds. Amsterdam: North-Holland.

Gifi, A. 1981. *Nonlinear multivariate analysis*. Leiden: Department of Data Theory.

Guttman, L. 1941. The quantification of a class of attributes: A theory and method of scale construction. In: *The Prediction of Personal Adjustment*, P. Horst et al, eds. New York: Social Science Research Council.

Meulman, J. 1982. *Homogeneity analysis of incomplete data*. Leiden: DSWO Press.

Wilkinson, J. H. 1965. *The algebraic eigenvalue problem*. Oxford: Clarendon Press.