

# Smacof at 50: A Manual

## Part 8: Homogeneity Analysis with Smacof

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### **Abstract**

smacofVO

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**Note:** This is a working manuscript which will be expanded/updated frequently. All suggestions for improvement are welcome. All Rmd, tex, html, pdf, R, and C files are in the public domain. Attribution will be appreciated, but is not required. The files can be found at <https://github.com/deleeuw> in the repositories smacofCode, smacofManual, and smacofExamples.

# 1 Introduction

## 1.1 Metric Unfolding

In metric unfolding we minimize a loss function of the form

$$\sigma(X, Y) = \sum_{i=1}^n \sum_{j=1}^m w_{ij} (\delta_{ij} - d(x_i, y_j))^2 \quad (1)$$

over the  $n \times p$  matrix  $X$  and the  $m \times p$  matrices  $Y$ . Both the weights  $W = \{w_{ij}\}$  and the dissimilarities  $\Delta = \{\delta_{ij}\}$  are known non-negative matrices.

The multidimensional unfolding model for preference judgments is often attributed to Clyde H. Coombs (1950), C. H. Coombs (1964), Kruskal and Carroll (1969), Roskam (1968)

## 1.2 Non-metric Unfolding

## 1.3 Simultaneous Non-Metric Unfolding

If we have data where the same individuals give preference judgments over multiple domains, or over the same domain on multiple occasions, or over the same domain with different experimental conditions, then we can use the loss function

$$\sigma(X, Y_1, \dots, Y_s) = \sum_{r=1}^s \sum_{i=1}^n \min_{\delta_i^r \in \Delta_i^r} \sum_{j=1}^{m_r} w_{ij}^r (\delta_{ij}^r - d(x_i, y_j^r))^2$$

Note that for each occasion there are different transformations  $\Delta_r$  and different matrices of column scores  $Y_r$ , but there is only a single matrix of row scores  $X$ .

$$y_j^r = \alpha_j^r y_r$$

## 1.4 Homogeneity Analysis

The Gifi System (Gifi (1990), Michailidis and De Leeuw (1998), De Leeuw and Mair (2009)) presents non-linear or non-metric versions of the classical linear multivariate analysis techniques (regression, analysis of variance, canonical analysis, discriminant analysis, principal component analysis) as special cases of Homogeneity Analysis, also known as Multiple Correspondence Analysis.

We give a somewhat non-standard introduction to homogeneity analysis here, to highlight the similarities with unfolding and the techniques we will present later on in this paper.

The data are a number of indicator matrices  $G_1, \dots, G_s$ . Indicator matrices are binary matrices, with rows that add up to one. They are used to code categorical variables. Rows corresponds with objects (or individuals), column with the categories (or levels) of a variable. An element  $g_{ij}$  is one in row  $i$  if object  $i$  is in category  $j$ , and all other elements in row  $i$  are zero.

Homogeneity analysis makes a joint maps in  $p$  dimensions of individuals and categories (both represented as points) in such a way that category points are close to the points for the individuals in the category. And, vice versa, individuals are close to the category points that they score in. If there is only one variable then it is trivial to make such a homogeneous map. We just make sure the individual points coincide with their category points. But there are  $s > 1$  indicator matrices, corresponding with  $s$  categorical variables, and the solution is a compromise trying to achieve homogeneity as well as possible for all variables simultaneously.

$$\sigma(X, Y_1, \dots, Y_s) = \sum_{r=1}^s \sum_{i=1}^n w_i^r d^2(x_i, y_i^r) = \sum_{r=1}^s \text{tr} (X - G_r Y_r)' W_r (X - G_r Y_r)$$

$$w_i^r := \sum_{j=1}^{m^r} g_{ij}^r w_{ij}^r$$

$$y_i^r := \sum_{j=1}^{m^r} g_{ij}^r y_j^r$$

Constraint is that  $\delta_{ij}^r$  is zero if  $i$  is in category  $j$  of variable  $r$ . There are no constraints on the other delta's in row  $i$ . of variable  $r$ . Thus we want an object to coincide with all  $s$  categories it is in.

star plot

$$Y_r = (G_r' W_r G_r)^{-1} G_r' W_r X$$

$$\min_Y \sigma(X, Y_1, \dots, Y_s) = \text{tr} X' \left\{ \sum_{r=1}^s \{W_r - W_r G_r (G_r' W_r G_r)^{-1} G_r' W_r\} \right\} X$$

$$X' W_* X = I$$

## 2 Loss Function

### 2.1 The Unconstrained Case

Now consider the closely related problem in which we do not require, as in homogeneity analysis, that

$$\delta_{i\star}^r := \sum_{j=1}^{m_r} g_{ij}^r \delta_{ij}^r = 0$$

but we merely require that  $\delta_{i\star}^r$  is less than or equal to all  $\delta_{ij}^r$  in row  $i$ . Formally

$$\delta_{i\star}^r \leq \delta_{ij}^r \quad \forall j = 1, \dots, m_r$$

or

$$g_{il}^r = 1 \Rightarrow \delta_{il}^r \leq \delta_{iv}^r \quad \forall v \neq \ell$$

$$\sigma(X, Y_1, \dots, Y_m) = \sum_{r=1}^s \left\{ \sum_{i=1}^n \sum_{\ell=1}^{k_r} w_{ij}^r (\delta_{i\ell}^r - d(x_i, y_\ell^r))^2 \right\}$$

In homogeneity analysis the geometric interpretation of loss is that we want individuals to coincide with the categories they score in (for all variables). The geometric interpretation of loss function ... is that we want individuals to be closer to the categories they score in than to the categories they do not score in (for all variables). The plot of the the  $k_r$  categories of variable  $r$  defines  $k_r$  Voronoi regions. The Voronoi region of category  $\ell$  is the polyhedral convex set of all points closer to category  $\ell$  than to any other category of variable  $r$ . The loss function ... vanishes if the  $x_i$  are all in the Voronoi regions of the categories they score in (for all variables).

Minimizing ... over the rows  $\delta_i^r$  is a monotone regression for a simple tree order. This is easily handled by using Kruskal's primary approach to ties (Kruskal (1964a), Kruskal (1964b), De Leeuw (1977)).

In stage 2 we do one or more metric smacof iterations for given  $\Delta_r$  to decrease the loss. These smacof iterations, or Guttman transforms, more or less ignore the fact that we are dealing with a rectangular matrix and use the weights to transform the problem into a symmetric one (as in Heiser and De Leeuw (1979)).

Thus for stage two purposes the loss function is

$$\sigma(Z_1, \dots, Z_m) = \sum_{r=1}^s \sum_{i=1}^{N_r} \sum_{j=1}^{N_r} w_{ij}^r (\delta_{ij}^r - d_{ij}(Z_r))^2,$$

with  $N_r := n + k_r$  and

$$Z_r := \begin{matrix} n \\ k_r \end{matrix} \begin{bmatrix} X \\ Y_r \end{bmatrix}^p.$$

The weights in  $W_r$  are now zero for the two diagonal blocks.

$$g_i^r := \begin{matrix} n \\ k_r \end{matrix} \begin{bmatrix} e_i \\ 0 \end{bmatrix}.$$

$$h_\ell^r := \begin{matrix} n \\ k_r \end{matrix} \begin{bmatrix} 0 \\ e_\ell \end{bmatrix}$$

so that  $x_i = Z_r' g_i^r$  and  $y_\ell^r = Z_r' h_\ell^r$ . It follows that

$$d^2(x_i, y_\ell^r) = \text{tr } Z_r' A_{i\ell}^r Z_r$$

where  $A_{i\ell}^r$ , of order  $n + k_r$ , is the rank-one, positive semi-definite, doubly centered matrix

$$A_{i\ell}^r := (g_i^r - h_\ell^r)(g_i^r - h_\ell^r)'$$

It further follows that

$$\sum_{i=1}^n \sum_{\ell=1}^{k_r} w_{i\ell}^r d^2(x_i, y_\ell^r) = \text{tr } Z_r' V_r Z_r,$$

where

$$V_r := \sum_{i=1}^n \sum_{\ell=1}^{k_r} w_{i\ell}^r A_{i\ell}^r,$$

so that  $V_r$  has the shape

$$V_r = \begin{matrix} & n & k_r \\ \begin{matrix} n \\ k_r \end{matrix} & \begin{bmatrix} \ddots & \square \\ \square & \ddots \end{bmatrix} \end{matrix}$$

with  $-W_r$  in the off-diagonal block, while the two diagonal blocks are diagonal matrices with the row and column sums of  $W_r$ .

In a similar way we define  $B_r(Z_r)$ , with the same shape as  $V_r$ , and with

$$B(Z_r) = \sum_{i=1}^n \sum_{\ell=1}^{k_r} w_{i\ell}^r \frac{\delta_{i\ell}^r}{d_{i\ell}(Z_r)} A_{i\ell}^r$$

$$\sigma(Z_1, \dots, Z_m) = \sum_{r=1}^s \{ \eta_r^2 - 2 \text{tr } Z_r' B(Z_r) Z_r + Z_r' V_r Z_r \}$$

with

$$\eta_r^2 := \sum_{i=1}^{N_r} \sum_{j=1}^{N_r} w_{ij}^r \{ \delta_{ij}^r \}^2$$

Define the Guttman transforms of  $Z_r$  as

$$\tilde{Z}_r = V_r^+ B(Z_r) Z_r$$

Then

$$\sigma_r(Z) := \eta_r^2 - 2\text{tr } Z'_r B(Z_r) Z_r + Z'_r V_r Z_r = \eta_r^2 - \eta^2(\tilde{Z}_r) + \text{tr } (Z_r - \tilde{Z}_r)' V_r (Z_r - \tilde{Z}_r)$$

If  $Z_r^{(k)}$  is  $Z_r$  at iteration  $k$  then

$$\text{tr } Z'_r B(Z_r) Z_r \geq \text{tr } Z'_r B(Z_r^{(k)}) Z_r^{(k)} = \text{tr } Z'_r V_r \tilde{Z}_r^{(k)}.$$

Thus

$$\sigma_r(Z) \leq \eta_r^2 - \eta^2(\tilde{Z}_r^{(k)}) + \text{tr } (Z_r - \tilde{Z}_r^{(k)})' V_r (Z_r - \tilde{Z}_r^{(k)})$$

It follows that in iteration  $k + 1$  we must minimize

$$\omega(Z_1, \dots, Z_s) := \sum_{r=1}^s \text{tr } (Z_r - \tilde{Z}_r^{(k)})' V_r (Z_r - \tilde{Z}_r^{(k)})$$

to compute the  $Z_r^{(k+1)}$ .

More explicitly we must minimize

$$\begin{aligned} \sum_{r=1}^s \text{tr } (X - \tilde{X}_r)' V_{11}^r (X - \tilde{X}_r) + 2 \sum_{r=1}^s \text{tr } (X - \tilde{X}_r)' V_{12}^r (Y_r - \tilde{Y}_r) + \\ \sum_{r=1}^s \text{tr } (Y_r - \tilde{Y}_r)' V_{22}^r (Y_r - \tilde{Y}_r) \end{aligned} \quad (2)$$

where  $\tilde{X}_r$  and  $\tilde{Y}_r$  are the two components of the Guttman transform  $\tilde{Z}_r$  of the current  $Z_r$ .

First minimize over  $Y_r$ , without constraints. This gives

$$Y_r = \tilde{Y}_r - \{V_{22}^r\}^{-1} V_{21}^r (X - \tilde{X}_r)$$

Substituting this in ... it remains to minimize

$$\sum_{r=1}^s \text{tr } (X - \tilde{X}_r)' V_{1|2}^r (X - \tilde{X}_r)$$

over  $X$ , where

$$V_{1|2}^r := V_{11}^r - V_{12}^r \{V_{22}^r\}^+ V_{21}^r$$

i.e. the Schur complement of  $V_{22}^r$  in  $V_r$ . If there are no constraints on  $X$  the solution is

$$X = \{V_{1|2}^r\}^+ \sum_{r=1}^s V_{1|2}^r \tilde{X}_r.$$

Because  $V_{1|2}^r$  is doubly-centered the solution  $X$  is column-centered.

## 2.2 Missing Data

## 2.3 Normalization of $X$

Constraint either (weak)

$$\text{tr } X' V_{1|2}^* X = 1$$

or (strong)

$$X' V_{1|2}^* X = I$$

Thus (weak)

$$X = \lambda \{V_{1|2}^*\}^{-1} \sum_{j=1}^m V_{1|2}^r \tilde{X}_r$$

with  $\lambda$  chosen such that ... is satisfied.

Or (strong)

$$X = \{V_{1|2}^*\}^{-\frac{1}{2}} K L'$$

(Procrustus)

In the unweighted case we have  $V_{11}^r = k_r I$ ,  $V_{22}^r = n I$ , and  $V_{12}^r = -E_{n \times k_r}$ . Thus  $V_{1|2}^r = k_r J_n$  and  $V_{1|2}^* = k_* J_n$  with  $J_n = I_n - n^{-1} E_{n \times n}$ , the centering matrix of order  $n$ .

The Guttman transform also simplifies in the unweighted case. The formulas were already given in Heiser and De Leeuw (1979).

## 2.4 Centroid Constraints on $Y$

$$Z_r = \begin{matrix} n \\ k_r \end{matrix} \begin{bmatrix} I \\ D_r^{-1} G_r' \end{bmatrix} X = H_r X$$

$$\sum_{j=1}^m Z_r' V_r Z_r = X' \left\{ \sum_{j=1}^m H_r' V_r H_r \right\} X.$$



### 3 Note

In order to not have to deal with general inverses and multiplications of gigantic symmetric matrices with largely empty diagonal blocks we solve the system

$$\begin{bmatrix} W_r & -W \\ -W' & W_c \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} P \\ Q \end{bmatrix}$$

for  $X$  and  $Y$ , with the known right hand side

$$\begin{bmatrix} P \\ Q \end{bmatrix} = \begin{bmatrix} B_r & -B \\ -B' & B_c \end{bmatrix} \begin{bmatrix} X^{(k)} \\ Y^{(k)} \end{bmatrix}$$

$W_r X - WY = P$  or  $X = W_r^{-1}(P + WY)$ . Substitute in  $W_c Y - W'X = Q$  to get  $W_c Y - W'W_r^{-1}(P + WY) = Q$  or  $(W_c - W'W_r^{-1}W)Y = Q + W'W_r^{-1}P$ .

Note that  $W_c - W'W_r^{-1}W$  is doubly-centered and  $Q + W'W_r^{-1}P$  is column-centered.

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