Smacof at 50
A Manual

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Abstract

TBD

Contents

Note: This is a working paper 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/smacofCode.

1 Introduction

In *Multidimensional Scaling (MDS)* the data consists of information about the similarity or dissimilarity between pairs of objects selected from a finite set $\mathcal{O} = \{o_1, \cdots, o_n\}$.

In *metric MDS* we have numerical dissimilarity measures and we want to map the objects o_i into n points x_i of some metric space in such a way that the distances between the points approximate the dissimilarities between the objects. In smacof the metric space is $\mathbb{R}^p$, the space of all p-tuples of real numbers, and in the code documented in this manual we assume the distance is the usual Euclidean distance. In *non-metric MDS* the information about the dissimilarities is incomplete. It is usually *ordinal*, i.e. it tells us in some way or another that some dissimilarties are larger or smaller than others. Somewhere between metric and non-metric MDS is MDS with *missing data*, in which some dissimilarities are known numbers while others are unknown. MDS with missing data is a form of *distance matrix completion* (Fang and O'Leary (2012)).

In the pioneering papers Kruskal (1964a) and Kruskal (1964b) the MDS problem was formulated for the first time as minimization of an explicit loss function, which measures the quality of the approximation of the dissimilarities by the distances. The loss function in least squares metric Euclidean MDS is called *raw stress* or *Kruskal's raw stress* and is defined as

$$\sigma(X) := \frac{1}{2}\sum w_{ij}(\delta_{ij} - d_{ij}(X))^2. \tag{1}$$

The symbol $:=$ is used for definitions. In definition (1) the w_{ij} are known non-negative *weights*, the δ_{ij} are the known non-negative *dissimilarities* between objects o_i and o_j, and the $d_{ij}(X)$ are the *distances* between the corresponding points x_i and x_j. The summation is over all $\binom{n}{2}$ pairs (i, j) with $j > i$, i.e. over elements below the diagonal of the matrices W and Δ. From now on we use "metric MDS" to mean Least Squares Metric Euclidean MDS.

The $n \times p$ matrix X, which has the coordinates x_i of the n points as its rows, is called the *configuration*, where p is the *dimension* of the Euclidean space in which we make the map. Thus

$$d_{ij}(X) = \sqrt{\sum_{s=1}^{p}(x_{is} - x_{js})^2}. \tag{2}$$

The metric MDS problem (of dimension p, for given W and Δ) is the minimization of (1) over the $n \times p$ configurations X.

The weights w_{ij} can be used to quantify information about the precision or importance of the corresponding dissimilarities. Some of the weights may be zero, which can be used to code *missing data*. If all weights are positive we have *complete data*. If we have complete data, and all weights are equal to one, we have *unweighted* metric MDS. Weights were only introduced in MDS in De Leeuw (1977), the pioneering papers by Shepard, Kruskal, and Guttman only consider the unweighted case.

We assume throughout that the weights are *irreducible* (De Leeuw (1977)). This means there is no partitioning of the index set $I_n := \{1, 2, \cdots, n\}$ into subsets for which all between-subset weights are zero. A reducible metric MDS problems decomposes into a number of smaller independent metric MDS problems, so the irreducibility assumption causes no real loss of generality.

The fact that the summation in (1) is over all $j < i$ indicates that the diagonal elements of Δ are not used (they are assumed to be zero) and the elements above the diagonal are not used as well (they are assumed to be equal to the corresponding elements below the diagonal). The somewhat mysterious factor $\frac{1}{2}$ in definition (1) is there because it simplifies some of the formulas in later sections of this paper.

Kruskal was not really interested in metric MDS and the "raw" loss function (1). His papers are really about non-metric MDS, by which we mean least squares non-metric Euclidean MDS. Non-metric MDS differs from metric MDS because we have incomplete information about the dissimilarities. As we have seen, that if some dissimilarities are missing metric MDS can handle this by using zero weights. In some situations, however, we only know the rank order of the non-missing dissimilarities. We do not know, or we refuse to use, their actual numeric values. Or, to put it differently, even if we have numerical dissimilarities we are looking for a *transformation* of the non-missing dissimilarities, where the transformation is chosen from a set of admissible transformations (for instance from all linear or monotone transformations). If the dissimilarities are non-numerical, for example rank orders or partitionings, we choose from the set of admissible *quantifications*.

In non-metric MDS the loss function becomes

$$\sigma(X, \widehat{D}) := \frac{1}{2} \sum w_{ij} (\hat{d}_{ij} - d_{ij}(X))^2, \tag{3}$$

where $\widehat{D}$ are now the quantified or transformed dissimilarities. In MDS parlance they are also called *pseudo-distances* or *disparities*. Loss function (3) must be minimized over both configurations and disparities, with the condition that the disparities $\widehat{D}$ are an admissible transformation of the dissimilarities Δ. In Kruskal's non-metric MDS this means requiring monotonicity. In this paper we will consider various other choices for the set of admissible transformations. We will use the symbol $\mathfrak{D}$ for the set of admissible transformations

The most familiar sets of admissible transformations (linear, polynomial, monotone) define convex cones with apex at the origin. This means that if $\widehat{D} \in \mathfrak{D}$ then so is $\lambda \widehat{D}$ for all $\lambda \geq 0$. But consequently minimizing (3) over all $\widehat{D} \in \mathfrak{D}$ and over all configurations has the trivial solution $\widehat{D} = 0$ and $X = 0$, corresponding with the global minimum $\sigma(X, \widehat{D}) = 0$. We need additional constraints to rule out this trivial solution, and in non-metric MDS this is done by choosing a *normalization* that keeps the solution away from zero.

Kruskal's solution is to normalize the raw stress by defining

$$\sigma(X,\Delta) := \frac{\sum w_{ij}(\hat{d}_{ij}-d_{ij}(X))^2}{\sum w_{ij}d_{ij}^2(X)}. \tag{4}$$

In fact in Kruskal's formulation there are no weights, and he actually takes the square root of (4) to define *Kruskal's stress*. The non-metric Euclidean MDS problem is to minimize loss function (4) over all $n \times p$ configurations X and all admissible disparities Δ.

1.1 Normalization

Normalization in non-metric MDS has been discussed in detail in Kruskal and Carroll (1969) and De Leeuw (1975). In the terminology of De Leeuw (1975) there are *explicit* and *implicit* normalizations.

In implicit normalization we minimize either

$$\sigma(X,\hat{D}) := \frac{\sum\sum_{1\leq j<i\leq n} w_{ij}(\hat{d}_{ij}-d_{ij}(X))^2}{\sum\sum_{1\leq j<i\leq n} w_{ij}\hat{d}_{ij}^2} \tag{5}$$

or

$$\sigma(X,\hat{D}) := \frac{\sum\sum_{1\leq j<i\leq n} w_{ij}(\hat{d}_{ij}-d_{ij}(X))^2}{\sum\sum_{1\leq j<i\leq n} w_{ij}d_{ij}^2(X)} \tag{6}$$

Kruskal (1964a) chooses definition (6) and calls the explicitly normalized loss function *normalized stress*. In fact, he takes the square root, which does not change the minimization problem, and only considers the unweighted case. Note that we overload the symbol σ to denote any one of the least squares loss functions. It will always be clear from the text which σ we are talking about.

In explicit normalization we minimize the raw stress $\sigma(X,\hat{D})$ from (3), but we add the constraint

$$\sum\sum_{1\leq j<i\leq n} w_{ij}d_{ij}^2(X) = 1, \tag{7}$$

or the constraint

$$\sum\sum_{1\leq j<i\leq n} w_{ij}\hat{d}_{ij}^2 = 1. \tag{8}$$

Kruskal and Carroll (1969) and De Leeuw (2019) show that these four normalizations all lead to essentially the same solution for X and $\hat{D}$, up to scale factors dictated by the choice of normalization. It is also possible to normalize both X and $\hat{D}$, either explicitly or implicitly, and again this will give the same solutions, suitably normalized. These invariance results assume the admissible transformations form a closed cone with apex at the origin, i.e. if $\hat{D}$ is admissible and $\lambda \geq 0$ then $\lambda\hat{D}$ is admissible as well. The matrices of Euclidean distances $D(X)$ form a similar closed cone as well. The LSNE-MDS problem is to find an element of the $\hat{D}$ cone and an element of the $D(X)$ cone where the angle between the two is a small as possible.

In the R version of smacof (De Leeuw and Mair (2009), Mair, Groenen, and De Leeuw (2022)) we use explicit normalization (8). This is supported by the result, also due to De Leeuw (1975), that projection on the intersection of the cone of disparities and the sphere defined by (8) is equivalent to first projecting on the cone and then normalizing the projection (see also Bauschke, Bui, and Wang (2018)).

In our version of non-metric MDS we need more flexibility. For algorithmic reasons that will become clear later on, we will go with the other explicit normalization (7) and minimize σ from (3) over normalized X and unnormalized $\widehat{D}$. For the final results the choice between (7) and (8) should not make a difference.

2 Some thoughts on ALS

I will take this opportunity to clear up some misunderstandings and confusions that have haunted the early development of non-metric MDS.

2.1 The Single-Phase approach

In Kruskal (1964a) defines

$$\sigma(X) := \min_{\widehat{D}\in\mathfrak{D}} \ \sigma(\widehat{D}, X) = \sigma(X, \widehat{D}(X)), \tag{9}$$

where $\sigma(\widehat{D}, X)$ is defined by (6). where the minimum is over admissible transformations. In definition (9)

$$\widehat{D}(X) := \underset{\widehat{D}\in\mathfrak{D}}{\text{argmin}}\, \sigma(X, \widehat{D}). \tag{10}$$

Normalized stress defined by (9) is now a function of X only. Under some conditions, which are true in Kruskal's definition of non-metric MDS,

$$\mathcal{D}\sigma(X) = \mathcal{D}_1\sigma(X, \widehat{D}(X)), \tag{11}$$

where $\mathcal{D}\sigma(X)$ are the derivatives of σ from (9) and $\mathcal{D}_1\sigma(X, \widehat{D}(X))$ are the partial derivatives of σ from (6) with respect to X. Thus the partials of σ from (9) can be computed by evaluating the partials of σ from (6) with respect to X at $(X, \widehat{D}(X))$. This has created much confusion in the past. The non-metric MDS problem is now to minimize σ from (9), which is a function of X alone.

Guttman (1968) calls this the *single-phase approach*. A variation of Kruskal's single-phase approach defines

$$\sigma(X) = \sum_{1\leq j<i\leq n}\sum w_{ij}(d^{\#}_{ij}(X) - d_{ij}(X))^2$$

where the $d^{\#}_{ij}(X)$ are *Guttman's rank images*, i.e. the permutation of the $d_{ij}(X)$ that makes them monotone with the δ_{ij} (Guttman (1968)). Or, alternatively, define

$$\sigma(X) := \sum_{1\leq j<i\leq n}\sum w_{ij}(d^{\%}_{ij}(X) - d_{ij}(X))^2$$

where the $\widehat{d}^{\%}_{ij}(X)$ are *Shepard's rank images*, i.e. the permutation of the δ_{ij} that makes them monotone with the $d_{ij}(X)$ (Shepard (1962a), Shepard (1962b), De Leeuw (2017b)).

Minimizing the Shepard and Guttman single-phase loss functions is computationally more complicated than Kruskal's *monotone regression* approach, mostly because the rank-image transformations are not differentiable, and there is no analog of (11) and of the equivalence of the different implicit and explicit normalizations.

2.2 The Two-Phase Approach

The *two-phase approach* or *alternating least squares (ALS)* approach alternates minimization of $\sigma(\widehat{D}, X)$ over X for our current best estimate of $\widehat{D}$ with minimization of $\sigma(\widehat{D}, X)$ over $\Delta \in \mathfrak{D}$ for our current best value of X. Thus an update from iteration k to iteration $k + 1$ looks like

$$\widehat{D}^{(k)} = \underset{\widehat{D}\in\mathfrak{D}}{\text{argmin}}\, \sigma(\widehat{D}, X^{(k)}), \tag{12}$$

$$X^{(k+1)} = \underset{X}{\text{argmin}}\, \sigma(\widehat{D}^{(k)}, X). \tag{13}$$

This ALS approach to MDS was in the air since the early (unsuccessful) attempts around 1968 of Young and De Leeuw to combine Torgerson's classic metric MDS method with Kruskal's monotone regression transformation. All previous implementations of non-metric smacof use the two-phase approach, and we will do the same in this paper.

As formulated, however, there are some problems with the ALS algorithm. Step (12) is easy to carry out, using monotone regression. Step (13) means solving a metric scaling problem, which is an iterative proces that requires an infinite number of iterations. Thus, in the usual implementations, step (12) is combined with one of more iterations of a convergent iterative procedure for metric MDS, such as smacof. If we take only one of these *inner iterations* the algorithm becomes indistinguishable from Kruskal's single-phase method. This has also created much confusion in the past.

In the usual implementations of the ALS approach we solve the first subproblem (12) exactly, while we take only a single step towards the solution for given $\widehat{D}$ in the second phase (13). If we have an infinite iterative procedure to compute the optimal $\widehat{D} \in \mathfrak{D}$ for given X, then a more balanced approach would be to take several inner iterations in the first phase and several inner iterations in the second phase. How many of each, nobody knows. In our current implementation of smacof we take several inner iteration steps in the first phase and a single inner iteration step in the second phase.

Notation and Terminology

We discuss some standard MDS notation, first introduced in De Leeuw (1977). This notation is useful for the second phase of the ALS algorithm, in which solve the metric MDS problem of we minimizing unnormalized $\sigma(X, \widehat{D})$ over X for fixed $\widehat{D}$. We will discuss the first ALS phase later in the paper.

Start with the unit vectors e_i of length n. They have a non-zero element equal to one in position i, all other elements are zero. Think of the e_i as the columns of the identity matrix.

Using the e_i we define for all $i \neq j$ the matrices

$$A_{ij} := (e_i - e_j)(e_i - e_j)'. \tag{14}$$

The A_{ij} are of order n, symmetric, doubly-centered, and of rank one. They have four non-zero elements. Elements (i,i) and (j,j) are equal to $+1$, elements (i,j) and (j,i) are -1.

The importance of A_{ij} in MDS comes from the equation

$$d_{ij}^2(X) = \text{tr}\ X'A_{ij}X. \tag{15}$$

In addition we use the fact that the A_{ij} form a basis for the $binomn2$-dimensional linear space of all doubly-centered symmetric matrices.

Expanding the square in the definition of stress gives

$$\sigma(X) = \frac{1}{2}\{\sum_{1\leq j<i\leq n}\sum w_k\delta_k^2 - 2\sum_{1\leq j<i\leq n}\sum w_k\delta_k d_k(X) + \sum_{1\leq j<i\leq n}\sum w_k d_k^2(X)\}. \tag{16}$$

It is convenient to have notation for the three separate components of stress from equation (16). Define

$$\eta_{\hat{D}}^2 = \sum_{1\leq j<i\leq n}\sum w_{ij}\hat{d}_{ij}^2, \tag{17}$$

$$\rho(X) = \sum_{1\leq j<i\leq n}\sum w_{ij}\hat{d}_{ij}d_{ij}(X), \tag{18}$$

$$\eta^2(X) = \sum_{1\leq j<i\leq n}\sum w_{ij}d_{ij}(X)^2. \tag{19}$$

which lead to

$$\sigma(X) = \frac{1}{2}\left\{\eta_{\hat{D}}^2 - 2\rho(X) + \eta^2(X)\right\}. \tag{20}$$

We also need

$$\lambda(X) = \frac{\rho(X)}{\eta(X)}. \tag{21}$$

Using the A_{ij} makes it possible to give matrix expressions for ρ and η^2. First

$$\eta^2(X) = \text{tr}\ X'VX, \tag{22}$$

with

$$V := \sum_{1\leq j<i\leq n}\sum w_{ij}A_{ij}. \tag{23}$$

In the same way

$$\rho(X) = \text{tr}\ X'B(X)X, \tag{24}$$

with

$$B(X) := \sum_{1\leq j<i\leq n}\sum w_{ij}\frac{\delta_{ij}}{d_{ij}(X)}A_{ij}. \tag{25}$$

Note that B is a function from the set of $n\times p$ configurations into the set of symmetric doubly-dentered matrices of order n. Because $B(X)$ and V are non-negative linear combinations of the A_{ij} they are both positive semi-definite. Because W is assumed to be irreducible the matrix V has rank

$n-1$, with only vectors proportional to the vector e with all elements equal to one in its null-space (De Leeuw (1977)).

Summarizing the results so far we have

$$\sigma(X)=\frac{1}{2}\{\eta_{\hat{D}}^{2}-\text{tr } X'B(X)X+\text{tr } X'VX\}. \tag{26}$$

Next we define the *Guttman transform* of a configuration X, for given W and Δ, as

$$G(X)=V^{+}B(X)X, \tag{27}$$

with V^{+} the Moore-Penrose inverse of V. In our computations we use

$$V^{+}=(V+\frac{1}{n}ee')^{-1}-\frac{1}{n}ee'$$

Also note that in the unweighted case with complete data $V=nJ$, where J is the centering matrix $I-\frac{1}{n}ee'$, and thus $V^{+}=\frac{1}{n}J$. The Guttman transform is then simply $G(X)=n^{-1}B(X)X$.

3 Smacof Loss

3.1 Derivatives

3.1.1 Lagrangian

3.1.2 Gradient

$$\mathcal{D}\sigma(X)=VX-B(X)X$$

3.1.3 Hessian

$$H_{st}(X)=\sum_{1\leq j<i\leq n}\sum w_{ij}\frac{\delta_{ij}}{d_{ij}^{3}(X)}(x_{is}-x_{js})(x_{it}-x_{jt})A_{ij}$$

$$\mathcal{D}_{st}\sigma(X)=\begin{cases}H_{st}(X) & \text{if } s\neq t,\\ V-B(X)+H_{st} & \text{if } s=t.\end{cases}$$

There are several ways to think of the Hessian. The simplest one (perhaps) is as an $np\times np$ symmetric matrix (corresponding to column-major R vector of length $\frac{1}{2}np(np+1)$). This is what we would use for a straightforward version of Newton-Raphson.

It is more elegant, however, to think of H as a symmetric super-matrix of order p, with as elements $n\times n$ matrices. And, for some purposes, such as the pseudo-confidence ellipsoids in De Leeuw (2017a), as a super-matrix of order n with as elements $p\times p$ matrices. Both the super-matrix interpretations lead to four-dimensional arrays, the first a $p\times p\times n\times n$ array, the second an $n\times n\times p\times p$ array. The different interpretations lead to different ways to store the Hessian in memory, and to different ways to retrieve its elements. Of course we can write routines to transform from one interpretation to another.

3.2 Stationary Points

4 Smacof Algorithm

4.1 Structure

4.1.1 Front End

4.1.2 Engine

4.1.3 Back End

4.2 Spline Basis Details

ninner m, degree k, order $d = k + 1$, nknots $m + 2d$, span $p = d + m$

B-splines

$B_{i,k}(x)$ is zero outside $[t_i, t_{i+k+1}]$

```
inner = c(.1, .5, .55, .9)
x = 0:10/10
print(x)
```

```
##  [1] 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
```

```
for (degree in 0:4) {
  ord <- degree + 1
  knots <- c(rep(0, ord), inner, rep(1, ord))
  a <- splineDesign(knots = knots, ord = ord, x = x)
  for (i in 1:11) {
    cat(formatC(x[i], digits = 2, format = "f"), " *** ",
        formatC(a[i, ], digits = 4, format = "f"), "\n")
  }
  cat("\n\n")
}
```

```
## 0.00  ***  1.0000 0.0000 0.0000 0.0000 0.0000
## 0.10  ***  0.0000 1.0000 0.0000 0.0000 0.0000
## 0.20  ***  0.0000 1.0000 0.0000 0.0000 0.0000
## 0.30  ***  0.0000 1.0000 0.0000 0.0000 0.0000
## 0.40  ***  0.0000 1.0000 0.0000 0.0000 0.0000
## 0.50  ***  0.0000 0.0000 1.0000 0.0000 0.0000
## 0.60  ***  0.0000 0.0000 0.0000 1.0000 0.0000
## 0.70  ***  0.0000 0.0000 0.0000 1.0000 0.0000
## 0.80  ***  0.0000 0.0000 0.0000 1.0000 0.0000
## 0.90  ***  0.0000 0.0000 0.0000 0.0000 1.0000
## 1.00  ***  0.0000 0.0000 0.0000 0.0000 1.0000
##
```

```
##
## 0.00  ***  1.0000 0.0000 0.0000 0.0000 0.0000 0.0000
## 0.10  ***  0.0000 1.0000 0.0000 0.0000 0.0000 0.0000
## 0.20  ***  0.0000 0.7500 0.2500 0.0000 0.0000 0.0000
## 0.30  ***  0.0000 0.5000 0.5000 0.0000 0.0000 0.0000
## 0.40  ***  0.0000 0.2500 0.7500 0.0000 0.0000 0.0000
## 0.50  ***  0.0000 0.0000 1.0000 0.0000 0.0000 0.0000
## 0.60  ***  0.0000 0.0000 0.0000 0.8571 0.1429 0.0000
## 0.70  ***  0.0000 0.0000 0.0000 0.5714 0.4286 0.0000
## 0.80  ***  0.0000 0.0000 0.0000 0.2857 0.7143 0.0000
## 0.90  ***  0.0000 0.0000 0.0000 0.0000 1.0000 0.0000
## 1.00  ***  0.0000 0.0000 0.0000 0.0000 0.0000 1.0000
##
##
## 0.00  ***  1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
## 0.10  ***  0.0000 0.8000 0.2000 0.0000 0.0000 0.0000 0.0000
## 0.20  ***  0.0000 0.4500 0.4944 0.0556 0.0000 0.0000 0.0000
## 0.30  ***  0.0000 0.2000 0.5778 0.2222 0.0000 0.0000 0.0000
## 0.40  ***  0.0000 0.0500 0.4500 0.5000 0.0000 0.0000 0.0000
## 0.50  ***  0.0000 0.0000 0.1111 0.8889 0.0000 0.0000 0.0000
## 0.60  ***  0.0000 0.0000 0.0000 0.6429 0.3413 0.0159 0.0000
## 0.70  ***  0.0000 0.0000 0.0000 0.2857 0.5714 0.1429 0.0000
## 0.80  ***  0.0000 0.0000 0.0000 0.0714 0.5317 0.3968 0.0000
## 0.90  ***  0.0000 0.0000 0.0000 0.0000 0.2222 0.7778 0.0000
## 1.00  ***  0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 1.0000
##
##
## 0.00  ***  1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
## 0.10  ***  0.0000 0.6400 0.3236 0.0364 0.0000 0.0000 0.0000 0.0000
## 0.20  ***  0.0000 0.2700 0.4946 0.2284 0.0069 0.0000 0.0000 0.0000
## 0.30  ***  0.0000 0.0800 0.3826 0.4818 0.0556 0.0000 0.0000 0.0000
## 0.40  ***  0.0000 0.0100 0.1627 0.6398 0.1875 0.0000 0.0000 0.0000
## 0.50  ***  0.0000 0.0000 0.0101 0.5455 0.4444 0.0000 0.0000 0.0000
## 0.60  ***  0.0000 0.0000 0.0000 0.2411 0.6748 0.0824 0.0018 0.0000
## 0.70  ***  0.0000 0.0000 0.0000 0.0714 0.5571 0.3238 0.0476 0.0000
## 0.80  ***  0.0000 0.0000 0.0000 0.0089 0.2752 0.4954 0.2205 0.0000
## 0.90  ***  0.0000 0.0000 0.0000 0.0000 0.0444 0.3506 0.6049 0.0000
## 1.00  ***  0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 1.0000
##
##
## 0.00  ***  1.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
## 0.10  ***  0.0000 0.5120 0.3928 0.0912 0.0040 0.0000 0.0000 0.0000 0.0000
## 0.20  ***  0.0000 0.1620 0.4228 0.3575 0.0569 0.0008 0.0000 0.0000 0.0000
## 0.30  ***  0.0000 0.0320 0.2219 0.5299 0.2038 0.0123 0.0000 0.0000 0.0000
## 0.40  ***  0.0000 0.0020 0.0524 0.4738 0.4093 0.0625 0.0000 0.0000 0.0000
## 0.50  ***  0.0000 0.0000 0.0009 0.2516 0.5499 0.1975 0.0000 0.0000 0.0000
## 0.60  ***  0.0000 0.0000 0.0000 0.0804 0.4606 0.4408 0.0180 0.0002 0.0000
## 0.70  ***  0.0000 0.0000 0.0000 0.0159 0.2413 0.5657 0.1613 0.0159 0.0000
## 0.80  ***  0.0000 0.0000 0.0000 0.0010 0.0691 0.4122 0.3952 0.1225 0.0000
## 0.90  ***  0.0000 0.0000 0.0000 0.0000 0.0049 0.1096 0.4149 0.4705 0.0000
## 1.00  ***  0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 1.0000
```

degree	order	ninner	nknots	span
0	1	4	6	5
1	2	4	8	6
2	3	4	10	7
3	4	4	12	8
4	5	4	14	9

$$\sum_i B_{i,k}(x) = 1$$

M-splines

$$M_{i,k}(x) = \frac{k+1}{t_{i+k+1} - t_i} B_{i,k}(X)$$

then

$$\int M_{i,k}(x)dx = 1$$

I-splines

$$I_{i,k+1}(z) = \int_{-\infty}^{z} M_{i,k}(x)dx$$

When is a B-spline increasing ?

$$\mathcal{D}B_{i,k}(x) =$$

Thus if

$$\mathcal{D}\sum_{i=1}^{d+m} \alpha_i B_{i,k}(x) =$$

It is sufficient that $\alpha_i \leq \alpha_{i+1}$

4.2.1 Ordinal MDS

4.2.2 Interval and Ratio MDS

4.2.3 The anchor and origin parameters

4.3 Cyclic Coordinate Descent

In the non-linear least squares (NNLS) problem the data are an $n \times p$ matrix X, a vector y with n elements, and a positive semi-definite diagonal matrix W. We want to minimize

$$\sigma(\beta) := \frac{1}{2}(X\beta - y)'W(X\beta - y)$$

over $\beta \geq 0$. In data analysis and statistics the problem is often solved by *active set methods*, implemented in R for example by NNLS (Mullen and van Stokkum (2023)) and FNNLS (Bro and De Jong (1997)). Active set methods are finitely convergent dual methods. While iterating the intermediate solutions are not feasible (i.e. non-negative). In fact in dual methods we reach feasibility and optimality at the same time. Also the number of iterations, although theoretically finite, can be very large.

In each smacof iteration we need an NNLS solution. Especially in the early iterations the solution does not have to be very precise. Also the solution from the previous NNLS problem will generally provide a very good starting value for the next iteration (each NNLS problem has a "hot start"). And finally, we would like all internediate solutions to be feasible. These considerations have lead us to using *cyclic coordinate descent* (CCD).

Suppose the current best feasible solution in CCD iteration k is $\beta^{(k)}$. The next CCD iteration changes each of the p coordinates of $\beta^{(k)}$ in turn, maintaining feasibility, while keeping the other $p-1$ coordinates fixed at their current values. Thus within a CCD iteration k we create intermediate solutions $\beta^{(k,1)}, \cdots, \beta^{(k,p)}$, where each of the intermediate solutions $\beta^{(k,r)}$ differs from the previous one $\beta^{(k,r-1)}$ in a single coordinate. For consistency we define $\beta^{(k,0)} := \beta^{(k)}$. After the iteration is finished we set $\beta^{(k+1)} = \beta^{(k,p)}$.

Note that in smacof each iteration modifies the coordinates in the order $1, \cdots, p$, which explains why the method is called "cyclic". There are variations of CCD in which the order within an iteration is random or greedy (choose the coordinate which gives the largest improvement) or zig-zag $1, \cdots, p, p-1, \cdots, 1$. We have not tried out these alternatives in smacf, but we may in the future.

The effect of changing a single coordinate on the loss function is

$$\sigma(\beta + \epsilon e_j) = \sigma(\beta) + \epsilon\, g_j(\beta) + \frac{1}{2}\epsilon^2 s_{jj},$$

where e_j is the unit vector corresponding with the coordinate we are changing, $g(\beta) := \mathcal{D}\sigma(\beta) = X'Wr(\beta)$ is the gradient at β, and $r(\beta) := X\beta - y$ is the residual. Also $S := X'WX$. Note that if $s_{jj} = 0$ then also $g_j(\beta) = 0$ and thus $\sigma(\beta + \epsilon e_j) = \sigma(\beta)$. In each CCD cycle we simply skip updating coordinate j.

If $s_{jj} > 0$ then $\sigma(\beta + \epsilon e_j)$ is a strictly convex quadratic in ϵ, which we must minimize under the constraint $\beta_j + \epsilon \geq 0$ or $\epsilon \geq -\beta_j$. Define $\hat{\epsilon}$ to be the solution of this constrained minimization problem.

The quadratic ... has its minimum at

$$\tilde{\epsilon} = -\frac{g_j(\beta)}{s_{jj}}$$

If $\beta + \tilde{\epsilon}$ is feasible then it is the update we are looking for. Thus $\hat{\epsilon} = \tilde{\epsilon}$. If $\beta + \tilde{\epsilon} < 0$ then the contrained minimum is attained at the boundary, i.e. $\hat{\epsilon} = -\beta_j$ and the updated β_j is zero. Thus, in summary, $\hat{\epsilon} = \max(\tilde{\epsilon}, -\beta_j)$.

One of the nice things about CCD is that

$$r(\hat{\beta}) = r(\beta) + \hat{\epsilon} x_j$$

$$g(\hat{\beta}) = g(\beta) + \hat{\epsilon} s_j$$

It follows that $\hat{\epsilon} = 0$ if and only if either $\beta_j = 0$ and $g_j(\beta) \geq 0$ or if $g_j(beta) = 0$ and $beta_j > 0$.

If $g_j(\beta) < 0$ then $\tilde{\epsilon} > 0$, and thus $\hat{\epsilon} > 0$ and $\sigma(\hat{\beta}) < \sigma(\beta)$. Thus we must have $g_j(\beta) \geq 0$.

If $\beta_j > 0$ and $g_j(\beta) \neq 0$ then there is an ϵ such that $\sigma(\beta + \epsilon e_j) < \sigma(\beta)$. Thus if $\beta_j > 0$ we must have $g_j(\beta) = 0$.

In summary at the minimum of σ over $\beta \geq 0$ we must have $\beta_j \geq 0$, $g_j(\beta) \geq 0$, and $\beta_j g_j(\beta) = 0$ for all j (*complementary slackness*).

$$\sigma(\beta + \epsilon e_j) = \sigma(\beta) + \epsilon\, g_j(\beta) + \frac{1}{2}\epsilon^2 s_{jj},$$

where $S := X'WX$.

Now suppose we minimize σ over $\beta \geq 0$.

Our best solution so far is $\beta^{(k)} \geq 0$. Minimize $\sigma(\beta^{(k)} + \epsilon e_1)$ over ϵ on the condition that $\beta_1^{(k)} + \epsilon \geq 0$ or $\epsilon \leq -\beta_1^{(k)}$. If $s_{11} = 0$ then also $g_1(\beta) = 0$ and we set $\beta^{(k+1,1)} = \beta^{(k,1)}$. If $s_{11} > 0$ we compute

$$\tilde{\epsilon} = -g_1(\beta)/s_{11}$$

If

$$\beta_1^{(k)} + \tilde{\epsilon} \geq 0$$

then

$$\beta^{(k+1,1)} = \beta_1^{(k)} + \tilde{\epsilon}$$

If

$$\beta_1^{(k)} + \tilde{\epsilon} < 0$$

we set

$$\beta^{(k+1,1)} = 0.$$

4.4 Majorization

Majorization, more recently better known as MM (Lange), minimize

Minimize σ over $x \in S$. Suppose there is a function η on $S \otimes S$ such that

1. $\sigma(x) \leq \eta(x, y)$ for all $x, y \in S$.
2. $\sigma(x) = \eta(x, x)$ for all $x \in S$.

The function η is called a *majorization scheme* for σ on S. A majorization scheme is *strict* if $\sigma(x) \leq \eta(x, y)$ for all $x, y \in S$ withj $x \neq y$.

Define

$$x^{(k+1)} = \underset{x \in S}{\text{argmin}}\, \eta(x, x^{(k)})$$

assuming that $\eta(x, y)$ attains its minimum over $x \in S$ for each y. Then

1. $\sigma(x^{(k+1)}) \leq \eta(x^{(k+1)}, x^{(k)})$ by ….
2. $\eta(x^{(k+1)}, x^{(k)}) \leq \eta(x^{(k)}, x^{(k)})$ by …
3. $\eta(x^{(k)}, x^{(k)}) = \sigma(x^{(k)})$ by …

a. If the minimum in … is attained for a unique x then $\eta(x^{(k+1)}, x^{(k)}) < \eta(x^{(k)}, x^{(k)})$
b. If the majorization is strict then $\sigma(x^{(k+1)}) < \eta(x^{(k+1)}, x^{(k)})$

4.5 Example

We give a small example in which we minimize σ with $\sigma(x) = \sqrt{x} - \log x$ over $x > 0$. Solving $\mathcal{D}\sigma(x) = 0$ gives $x = 4$ as the solution we are looking for.

To arrive at this solution using majorization we start with

$$\sqrt{x} \leq \sqrt{y} + \frac{1}{2}\frac{x - y}{\sqrt{y}},$$

which is true because a differentiable concave function such as the square root is majorized by its tangent everywhere. Inequality … implies

$$\sigma(x) \leq \eta(x, y) = \sqrt{y} + \frac{1}{2}\frac{x - y}{\sqrt{y}} - \log x.$$

Now $\mathcal{D}_1\eta(x, y) = 0$ if and only if $x = 2\sqrt{y}$ and thus the majorization algorithm is

$$x^{(k+1)} = 2\sqrt{x^{(k)}}$$

The sequence $x^{(k)}$ converges monotonically to the fixed point $x = 2\sqrt{x}$, i.e. to $x = 4$. If $x^{(0)} < 4$ the sequence is increasing, if $x^{(0)} < 4$ it is decreasing. Also, by l'Hôpital,

$$\lim_{x \to 4} \frac{2\sqrt{x} - 4}{x - 4} = \frac{1}{2}$$

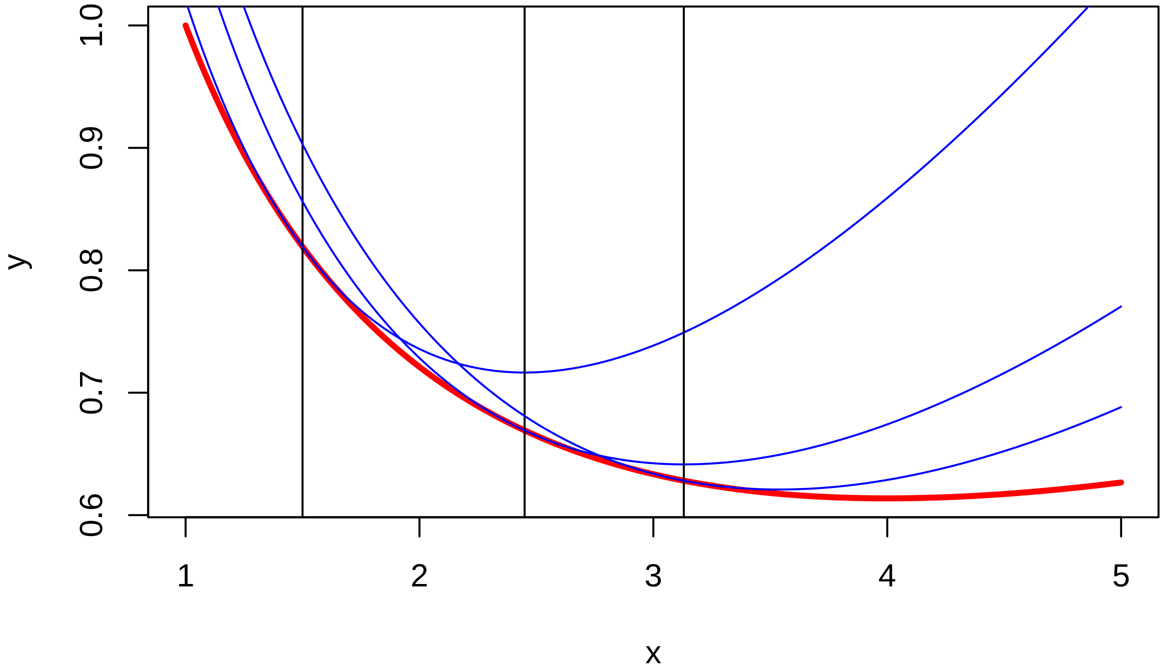
and thus convergence to the minimizer is linear with asymptotic convergence rate $\frac{1}{2}$. By another application of l'Hôpital

$$\lim_{x\rightarrow 4}\frac{\sigma(2\sqrt{x}))-\sigma(4)}{\sigma(x)-\sigma(4)}=\frac{1}{4},$$

and convergence to the minimum is linear with asymptotic convergence rate $\frac{1}{4}$. Linear convergence to the minimizer is typical for majorization algorithms, as is the twice-as-fast linear convergence to the minimum value.

In table ... we show convergence starting at $x = 1.5$.

```
## itel   1 2.5000000000 0.2055741244
## itel   2 1.5505102572 0.0554992066
## itel   3 0.8698308399 0.0144357214
## itel   4 0.4615431837 0.0036822877
## itel   5 0.2378427379 0.0009299530
## itel   6 0.1207437506 0.0002336744
## itel   7 0.0608344795 0.0000585677
## itel   8 0.0305337787 0.0000146606
## itel   9 0.0152961358 0.0000036675
## itel  10 0.0076553935 0.0000009172
## itel  11 0.0038295299 0.0000002293
## itel  12 0.0019152235 0.0000000573
## itel  13 0.0009577264 0.0000000143
## itel  14 0.0004788919 0.0000000036
## itel  15 0.0002394531 0.0000000009
```



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