Global Minima by Penalized Full-dimensional Scaling

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Abstract

The full-dimensional (metric, Euclidean, least squares) multidimensional scaling stress loss function is combined with a quadratic external penalty function term. The trajectory of minimizers of stress for increasing values of the penalty parameter is then used to find (tentative) global minima for low-dimensional multidimensional scaling. This is illustrated with several one-dimensional and two-dimensional examples.

Contents

Note: This is a working paper which will be expanded/updated frequently. All suggestions for improvement are welcome. The directory deleeuwpdx.net/pubfolders/penalty has a pdf version, a html version, the bib files, the complete Rmd file with the code chunks, and the R source code.

Introduction

Full-dimensional Scaling (FDS) was introduced by De Leeuw (1993). De Leeuw, Groenen, and Mair (2016) discuss it in some detail. In FDS we minimize the usual Multidimensional Scaling (MDS) least squares loss function first used by Kruskal (1964a) and Kruskal (1964b).

$$\sigma(Z)=\frac{1}{2}\mathop{\sum\sum}_{1\leq i<j\leq n}w_{ij}(\delta_{ij}-d_{ij}(Z))^2 \tag{1}$$

over all $n\times n$ *configuration matrices* Z. The loss at Z is often called the *stress* of configuration Z. More generally we define pMDS as the problem of minimizing (1) over all $n\times p$ matrices. Thus FDS is the same as nMDS. If a configuration Z has n columns (i.e. is square) it is called a *full configuration*.

In (1) the matrices $W=\{w_{ij}\}$ and $\Delta=\{\delta_{ij}\}$ of *weights* and *dissimilarities* are non-negative, symmetric, and hollow. To simplify matters we suppose both W and Δ have positive off-diagonal elements. The matrix $D(X)=\{d_{ij}(Z)\}$ has the *Euclidean distances* between the rows of the configuration Z. Thus

$$d_{ij}(Z)=\sqrt{(z_i-z_j)'(z_i-z_j)}.$$

We now introduce some standard MDS notation, following De Leeuw (1977). Define the matrix $V=\{v_{ij}\}$ by

$$v_{ij}=\begin{cases}-w_{ij}&\text{if }i\neq j,\\ \sum_{j=1}^n w_{ij}&\text{if }i=j,\end{cases} \tag{2}$$

and the matrix valued function $B(Z)=\{b_{ij}(Z)\}$ by

$$b_{ij}(Z)=\begin{cases}-w_{ij}e_{ij}(Z)&\text{if }i\neq j,\\ \sum_{j=1}^n w_{ij}e_{ij}(Z)&\text{if }i=j,\end{cases} \tag{3}$$

where $E(Z) = \{e_{ij}(Z)\}$ is defined as

$$e_{ij}(Z) = \begin{cases} \frac{\delta_{ij}}{d_{ij}(Z)} & \text{if } d_{ij}(Z) > 0, \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

Note that V and $B(Z)$ are both positive semi-definite and doubly-centered. Matrix V has rank $n-1$. If all off-diagonal $d_{ij}(Z)$ are positive then $B(Z)$ has rank $n-1$ for all Z. Note that De Leeuw (1984) established that near a local minimum of stress all off-diagonal distances are indeed positive. The only vectors in the null-space of both V and $B(Z)$ are the vectors proportional to the vector with all elements equal to one.

We assume in addition, without loss of generality, that

$$\frac{1}{2}\sum\sum_{1\leq i<j\leq n} w_{ij}\delta_{ij}^2 = 1.$$

With these definitions we can rewrite the stress (1) as

$$\sigma(Z) = 1 - \mathbf{tr}\ Z'B(Z)Z + \frac{1}{2}\mathbf{tr}\ Z'VZ, \tag{5}$$

and we can write the stationary equations as

$$(V - B(Z))Z = 0, \tag{6}$$

or, in fixed point form, $Z = V^+B(Z)Z$.

Equation (5) shows, by the way, something which is already obvious from (1). Distances are invariant under translation. This is reflected in $B(Z)$ and V being doubly-centered. As a consequence we usually require, again without loss of generality, that Z is column-centered. And that implies that Z has rank at most $n-1$, which means that FDS is equivalent to minimizing stress over all $n \times (n-1)$ matrices, which we can assume to be column-centered as well. Configurations with $n-1$ columns can be called full configurations as well. In addition, distances are invariant under rotation, and consequently if Z solves the stationary equations with value $\sigma(Z)$ then ZK solves the stationary equations for all rotation matrices K, and $\sigma(ZK) = \sigma(K)$. This means there are no isolated local minima in configuration space, each local minimum is actually a continuum of rotated matrices in $\mathbb{R}^{n\times n}$. This is a nuisance in the analysis of FDS and pMDS that is best dealt with by switching to the parametrization outlined in De Leeuw (1993).

Convex FDS

Instead of defining the loss function (1) on the space of all $n \times n$ configuration matrices Z we can also define it over the space of all positive semidefinite matrices C of order n. This gives

$$\sigma(C) = 1 - \sum\sum_{1\leq i<j\leq n} w_{ij}\delta_{ij}\sqrt{c_{ii} + c_{jj} - 2c_{ij}} + \frac{1}{2}\mathbf{tr}\ VC. \tag{7}$$

The Convex Full-dimensional Scaling (CFDS) problem is to minimize loss function (7) over all $C \gtrsim 0$. Obviously if Z minimizes (1) then $C = ZZ'$ minimizes (7). And, conversely, if C minimizes (7) then any Z such that $C = ZZ'$ minimizes (1).

The definition (7) shows that the CFDS loss function is a convex function on the cone of positive semi-definite matrices, because the square root of a non-negative linear function of the elements of C is concave. Positivity of the weights and dissimilarities implies that loss is actually strictly convex. The necessary and sufficient conditions for C to be the unique solution of the CFDS problem are simply the conditions for a proper convex function to attain its minimum at C on a closed convex cone (Rockafellar (1970), theorem 31.4).

$$\begin{aligned} V - B(C) &\gtrsim 0, \\ C &\gtrsim 0, \\ \mathbf{tr}\ C(V - B(C)) &= 0. \end{aligned}$$

The conditions say that C and $V - B(C)$ must be positive semi-definite and have complimentary null spaces.

By the same reasoning as in the full configuration case, we also see that CFDS is equivalent to maximizing (7) over all doubly-centered positive semi-definite matrices.

If C is the solution of the CFDS problem then $\mathbf{rank}(C)$ is called the *Gower rank* of the MDS problem defined by W and Δ (De Leeuw (2016)). Although there is a unique Gower rank associated with each CFDS problem, we can also talk about the *approximate Gower rank* by ignoring the small eigenvalues of C.

FDS using SMACOF

The usual SMACOF algorithm can be applied to FDS as well. The iterations start with $Z^{(0)}$ and use the update rule

$$Z^{(k+1)} = V^{+}B(Z^{(k)})Z^{(k)}, \tag{8}$$

where V^{+} is the Moore-Penrose inverse of V, and is consequently also doubly-centered. This means that all $Z^{(k)}$ in the SMACOF sequence, except possibly $Z^{(0)}$, are column-centered and of rank at most $n-1$. Equation (8) also shows that if $Z^{(0)}$ is of rank $p < n-1$ then all $Z^{(k)}$ are of rank p as well.

De Leeuw (1977) shows global convergence of the SMACOF sequence for pMDS, generated by (8), to a stationary point, i.e. a point satisfying $(V - B(Z))Z = 0$. This result also applies, of course, to nMDS, i.e. FDS. If Z is a solution of the stationary equations then with $C = ZZ'$ we have both $(V - B(C))C = 0$ and $C \gtrsim 0$, but since we generally do not have $V - B(Z) \gtrsim 0$, this does not mean that C solves the CFDS problem.

In fact, suppose the unique CMDS solution has Gower rank $r \geq 2$. Start the SMACOF FDS iterations (8) with $Z^{(0)}$ of the form $Z^{(0)} = \begin{bmatrix} X^{(0)} & \mid & 0 \end{bmatrix}$, where $X^{(0)}$ is an $n \times p$ matrix of rank $p < r$. All $Z^{(k)}$ will be of this form and will also be of rank p, and all accumulation points Z of the SMACOF sequence will have this form and $\mathbf{rank}(Z) \leq p$. Thus $C = ZZ'$ cannot be the solution of the CMDS problem.

The next result shows that things are allright, after all. Although stress in FDS is certainly not a convex function of Z, it remains true that all local minima are global.

Lemma 1: [Expand] If FDS stress has a local minimum at $\begin{bmatrix} X & \mid & 0 \end{bmatrix}$, where X is $n \times p$ and the zero block is $n \times q$ with $q > 1$, then

1: $\mathcal{D}\sigma(X) = (V - B(X))X = 0$.

2: $\mathcal{D}^2\sigma(X) \gtrsim 0$.

3: $V - B(X) \gtrsim 0$.

Proof: We use the fact that stress is differentiable at a local minimum (De Leeuw (1984)). If $Z = \begin{bmatrix} X & \mid & 0 \end{bmatrix} + \epsilon \begin{bmatrix} P & \mid & Q \end{bmatrix}$ then we must have $\sigma(Z) \geq \sigma(X)$ for all P and Q. Now

$$\sigma(Z) = \sigma(X) + \epsilon \text{ tr } P'\mathcal{D}\sigma(X) + \\ + \frac{1}{2}\epsilon^2\ \mathcal{D}^2\sigma(X)(P,P) + \frac{1}{2}\epsilon^2 \text{ tr } Q'(V - B(X))Q + o(\epsilon^2). \quad (9)$$

The lemma follows from this expansion. ■

Theorem 1: [FDS Local Minima] If stationary point Z of FDS is a local minimum, then it also is the global minimum, and $C = ZZ'$ solves the CFDS problem.

Proof: We start with a special case. Suppose Z is a doubly-centered solution of the FDS stationary equations with $\mathbf{rank}(Z) = n - 1$. Then $(V - B(Z))Z = 0$ implies $V = B(Z)$, which implies $\delta_{ij} = d_{ij}(Z)$ for all i, j. Thus $\sigma(Z) = 0$, which obviously is the global minimum.

Now suppose Z is a doubly-centered local minimum solution of the FDS stationary equations with $\mathbf{rank}(Z) = r < n - 1$. Without loss of generality we assume Z is of the form $Z = \begin{bmatrix} X & \mid & 0 \end{bmatrix}$, with X an $n \times r$ matrix of rank r. For $C = ZZ'$ to be a solution of the CFDS problem it is necessary and sufficient that $V - B(Z) \gtrsim 0$. Lemma 1 shows that this is indeed the case at a local minimum. ■

Corrollary 1: [Saddle] A pMDS solution of the stationary equations with Z singular is a saddle point.

Corrollary 2: [Nested] Solutions of the stationary equations of pMDS are saddle points of qMDS with $q > p$.

The proof of lemma 1 shows that for any $n \times p$ configuration Z, not just for solutions of the FDS stationary equations, if $V - B(Z)$ is indefinite we can decrease loss by adding another dimension. If Z is a stationary point and $V - B(Z)$ is positive semi-definite then we actually have found the CFDS solution, the Gower rank, and the global minimum (De Leeuw (2014)).

Penalizing Dimensions

In Shepard (1962a) and Shepard (1962b) a nonmetric multidimensional scaling technique is developed which minimizes a loss function over configurations in full dimensionality $n - 1$. In that sense the technique is similar to FDS. Shepard's iterative process aims to maintain monotonicity between distances and dissimilarities and at the same time concentrate as much of the variation as possible in a small number of dimensions (De Leeuw (2017)).

Let us explore the idea of concentrating variation in $p < n-1$ dimensions, but use an approach which is quite different from the one used by Shepard. We remain in the FDS framework, but we aim for solutions in $p < n-1$ dimensions by penalizing $n-p$ dimensions of the full configuration, using the classical Courant quadratic penalty function.

Partition a full configuration $Z = \begin{bmatrix} X & \mid & Y \end{bmatrix}$, with X of dimension $n \times p$ and Y of dimension $n \times (n-p)$. Then

$$\sigma(Z) = 1 - \mathbf{tr}\ X'B(Z)X - \mathbf{tr}\ Y'B(Z)Y + \frac{1}{2}\mathbf{tr}\ X'VX + \frac{1}{2}\mathbf{tr}\ Y'VY. \tag{10}$$

Also define the *penalty term*

$$\tau(Y) = \frac{1}{2}\mathbf{tr}\ Y'VY, \tag{11}$$

and *penalized stress*

$$\pi(Z, \lambda) = \sigma(Z) + \lambda\ \tau(Y). \tag{12}$$

Our proposed method is to minimize penalized stress over Z for a sequence of values $0 = \lambda_1 < \lambda_2 < \cdots < \lambda_m$. For $\lambda = 0$ this is simply the FDS problem, for which we know we can compute the global minimum. For fixed $0 < \lambda < +\infty$ this is a Penalized FDS or PFDS problem. PFDS problems with increasing values of λ generate a *trajectory* $Z(\lambda)$ in configuration space.

The general theory of exterior penalty functions, which we review in appendix A of this paper, shows that increasing λ leads to an increasing sequence of stress values σ and a decreasing sequence of penalty terms τ. If $\lambda \rightarrow +\infty$ we approximate the global minimum of the FDS problem with Z of the form $Z = \begin{bmatrix} X & \mid & 0 \end{bmatrix}$, i.e. of the pMDS problem. This assumes we do actually compute the global minimum for each value of λ, which we hope we can do because we start at the FDS global minimum, and we slowly increase λ. There is also a local version of the exterior penalty result, which implies that $\lambda \rightarrow \infty$ takes us to a local minimum of pMDS, so there is always the possibility of taking the wrong trajectory to a local minimum of pMDS.

Local Minima

The stationary equations of the PFDS problem are solutions to the equations

$$(V - B(Z))X = 0, \tag{13}$$

$$((1+\lambda)V - B(Z))Y = 0. \tag{14}$$

We can easily related stationary points and local minima of the FDS and PFDS problem.

Theorem 2: [PFDS Local Minima]

1: If X is a stationary point of the pMDS problem then $Z = [X \mid 0]$ is a stationary point of the PFDS problem, no matter what λ is.

2: If $Z = [X \mid 0]$ is a local minimum of the PFDS problem then X is a local minimum of pMDS and $(1+\lambda)V - B(X) \gtrsim 0$, or $\lambda \geq \|V^+B(X)\|_\infty - 1$, with $\| \bullet \|_\infty$ the spectral radius (largest eigenvalue).

Proof:

Part 1 follows by simple substitution in the stationary equations.

Part 2 follows from the expansion for $Z = [X + \epsilon P \mid \epsilon Q]$.

$$\pi(Z) = \pi(X) + \epsilon \text{ tr } P'\mathcal{D}\sigma(X) + \\ + \frac{1}{2}\epsilon^2 \ \mathcal{D}^2\sigma(X)(P,P) + \frac{1}{2}\epsilon^2 \text{ tr } Q'((1+\lambda)V - B(X))Q + o(\epsilon^2). \tag{15}$$

At a local minimum we must have $\mathcal{D}\sigma(X) = 0$ and $\mathcal{D}^2\sigma(X)(P,P) \gtrsim 0$, which are the necessary conditions for a local minimum of pMDS. We also must have $((1+\lambda)V - B(X)) \gtrsim 0$. ■

Note that the conditions in part 2 of theorem 2 are also sufficient for PFDS to have a local minimum at $[X \mid 0]$, provided we eliminate translational and rotational indeterminacy by a suitable reparametrization, as in De Leeuw (1993).

Algorithm

The SMACOF algorithm for penalized stress is a small modification of the unpenalized FDS algorithm (8). We start our iterations for λ_j with the solution for λ_{j-1} (the starting solution for $\lambda_1 = 0$ can be completely arbitrary). The update rules for fixed λ are

$$X^{(k+1)} = V^+B(Z^{(k)})X^{(k)}, \tag{16}$$

$$Y^{(k+1)} = \frac{1}{1+\lambda}V^+B(Z^{(k)})Y^{(k)}. \tag{17}$$

Thus we compute the FDS update $Z^{(k+1)} = V^+B(Z^{(k)})Z^{(k)}$ and then divide the last $n-p$ columns by $1+\lambda$.

Code is in the appendix. Let us analyze a number of examples.

Examples

This section has a number of two-dimensional and a number of one-dimensional examples. The one-dimensional examples are of interest, because of the documented large number of local minima of stress in the one-dimensional case, and the fact that for small and medium n exact solutions are available (for example, De Leeuw (2005)). By default we use `seq(0, 1, length = 101)` for λ in most examples, but for some of them we dig a bit deeper and use longer sequences with smaller increments.

If for some value of λ the penalty term drops below the small cutoff γ, for example 10^{-10}, then there is not need to try larger values of λ, because they will just repeat the same result. We hope that result is the global minimum of the 2MDS problem.

The output for each example is a table in which we give, the minimum value of stress, the value of the penalty term at the minimum, the value of λ, and the number of iterations needed for convergence. Typically we print for the first three, the last three, and some regularly spaced intermediate values of λ. Remember that the stress values increase with increasing λ, and the penalty values decrease.

For two-dimensional examples we plot all two-dimensional configurations, after rotating to optimum match (using the function `matchMe()` from the appendix). We connect corresponding points for different values of λ. Points corresponding to the highest value of λ are labeled and have a different plot symbol. For one-dimensional examples we put `1:n` on the horizontal axes and plot the single dimension on the vertical axis, again connecting corresponding points. We label the points corresponding with the highest value of λ, and draw horizontal lines through them to more clearly show their order on the dimension.

The appendix also has code for the function `checkUni()`, which we have used to check the solutions in the one dimensional case are indeed local minima. The function checks the necessary condition for a local minimum $x = V^{+}u$, with

$$u_i = \sum_{j=1}^{n} w_{ij}\delta_{ij}\ \textbf{sign}\ (x_i - x_j).$$

It should be emphasized that all examples are just meant to study performance and convergence of penalized FDS. There is no interpretation of the MDS results

Chi Squares

In this example, of order 10, the δ_{ij} are square roots of independent draws from a central chi-square distribution with two degrees of freedom. We use a fixed seed for the random number generator.

If we analyze the data with smacof in two dimensions, using the Torgerson initial configuration, we find a stress of 0.0862287021 after 65 iterations. All smacof runs in this paper have a maximum number of iterations of 10,000 and stop if the difference between successive stress values is less than 1e-10. A full-dimensional scaling with $p = 9$ gives stress 0.0730261617 after 198 iterations. The singular values of the full dimensional solution are

```
## [1] +0.322688 +0.207891 +0.163634 +0.096146 +0.045038 +0.000001 +0.000000
## [8] +0.000000 +0.000000
```

and thus the Gower rank of these data is five.

We can also start our smacof iterations with the first two dimensions of the full dimensional solution. Stress is 0.0862287021 after 62 iterations, the same solution as with the Torgerson start.

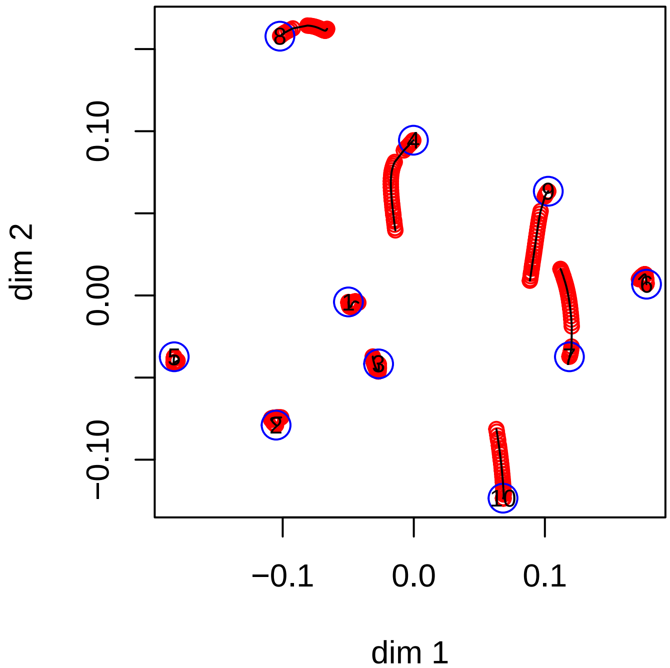
If we run smacof 1000 times with a random start we find five different local minima, and the one with the smallest stress is found in about 40% of the cases. Again, this is the Torgerson solution.

```
##
## 0.0862287 0.0955797 0.0990518 0.0995697  0.100125
##       394       246       174        69       117
```

We now apply our global optimization method, using 101 values of λ, equally spaced between zero and one. Again we converge on the Torgerson solution, which by all indications is the global minimum of stress for these data.

```
## itel  203 lambda   0.000000 stress 0.073026 penalty 0.422435
## itel    4 lambda   0.010000 stress 0.073054 penalty 0.091005
## itel    3 lambda   0.020000 stress 0.073141 penalty 0.086529
## itel    2 lambda   0.030000 stress 0.073269 penalty 0.082545
## itel    1 lambda   0.040000 stress 0.073390 penalty 0.079778
## itel    2 lambda   0.050000 stress 0.073688 penalty 0.074219
## itel    1 lambda   0.060000 stress 0.073899 penalty 0.071053
## itel    1 lambda   0.070000 stress 0.074170 penalty 0.067522
## itel    1 lambda   0.080000 stress 0.074497 penalty 0.063768
## itel    1 lambda   0.090000 stress 0.074874 penalty 0.059891
## itel    1 lambda   0.100000 stress 0.075299 penalty 0.055962
## itel    1 lambda   0.110000 stress 0.075765 penalty 0.052032
## itel    1 lambda   0.120000 stress 0.076269 penalty 0.048144
## itel    1 lambda   0.130000 stress 0.076806 penalty 0.044331
## itel    1 lambda   0.140000 stress 0.077368 penalty 0.040621
## itel    1 lambda   0.150000 stress 0.077951 penalty 0.037038
## itel    1 lambda   0.160000 stress 0.078548 penalty 0.033601
## itel    1 lambda   0.170000 stress 0.079152 penalty 0.030322
## itel    1 lambda   0.180000 stress 0.079756 penalty 0.027213
## itel    1 lambda   0.190000 stress 0.080355 penalty 0.024279
## itel    1 lambda   0.200000 stress 0.080942 penalty 0.021526
## itel    1 lambda   0.210000 stress 0.081511 penalty 0.018955
## itel    1 lambda   0.220000 stress 0.082058 penalty 0.016567
## itel    1 lambda   0.230000 stress 0.082578 penalty 0.014364
## itel    1 lambda   0.240000 stress 0.083067 penalty 0.012345
## itel    9 lambda   0.250000 stress 0.085317 penalty 0.003278
## itel    2 lambda   0.260000 stress 0.085541 penalty 0.002404
## itel    2 lambda   0.270000 stress 0.085724 penalty 0.001723
## itel    3 lambda   0.280000 stress 0.085924 penalty 0.001009
## itel    2 lambda   0.290000 stress 0.086017 penalty 0.000689
## itel    3 lambda   0.300000 stress 0.086111 penalty 0.000374
## itel    4 lambda   0.310000 stress 0.086177 penalty 0.000158
## itel    3 lambda   0.320000 stress 0.086202 penalty 0.000080
## itel    4 lambda   0.330000 stress 0.086218 penalty 0.000031
```

```
## itel     6 lambda   0.340000 stress 0.086226 penalty 0.000007
## itel     8 lambda   0.350000 stress 0.086228 penalty 0.000001
```



Regular Simplex

The regular simplex has all dissimilarities equal to one. We use an example with $n = 10$, for which the global minimum (as far as we know) of pMDS with $p = 2$ is a configuration with nine points equally spaced on a circle and one point in the center.

Using the Torgerson initial configuration in two dimensions, smacof finds a stress of 0.1110521776 after 872 iterations. This corresponds with the presumed global minimum.

A full-dimensional scaling with $p = 9$ gives stress $1.8681520461 \times 10^{-31}$ after 1 iterations. The singular values of the full dimensional solution are

```
## [1] +0.149071 +0.149071 +0.149071 +0.149071 +0.149071 +0.149071 +0.149071
## [8] +0.149071 +0.149071
```

and thus the Gower rank of these data is six.

If we our smacof iterations with the first two dimensions of the full dimensional solution stress is 0.1110521776 after 872 iterations, the same global solution as with the Torgerson start.

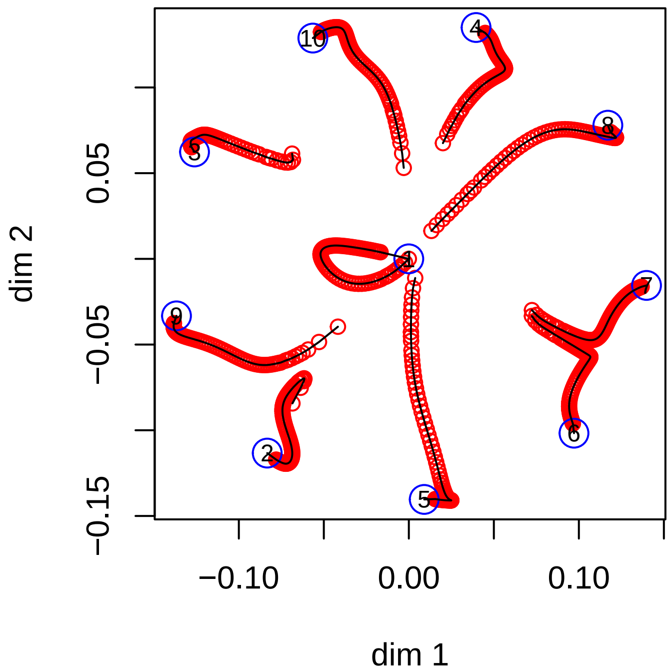
If we run smacof 1000 times with a random start we find three different local minima, and the one with the smallest stress is found in about 70% of the cases. Again, this is the global solution. There are, of course, many more local minima, because each permutation of the 10 solution points will give another local minimum with the same stress value.

```
##
```

```
##  0.10988 0.111052 0.111058
##      715      284        1
```

Our global optimization method with the default λ sequence also converges on the global solution.

```
## itel    1 lambda   0.000000 stress 0.000000 penalty 0.400000
## itel    7 lambda   0.010000 stress 0.000103 penalty 0.375240
## itel    5 lambda   0.020000 stress 0.000427 penalty 0.360212
## itel    3 lambda   0.030000 stress 0.000916 penalty 0.346937
## itel    2 lambda   0.040000 stress 0.001533 penalty 0.334923
## itel    2 lambda   0.050000 stress 0.002378 penalty 0.321650
## itel    2 lambda   0.060000 stress 0.003468 penalty 0.307513
## itel    2 lambda   0.070000 stress 0.004816 penalty 0.292842
## itel    1 lambda   0.080000 stress 0.005905 penalty 0.283148
## itel    1 lambda   0.090000 stress 0.007178 penalty 0.272814
## itel    2 lambda   0.100000 stress 0.009438 penalty 0.255499
## itel    1 lambda   0.110000 stress 0.011002 penalty 0.245389
## itel    1 lambda   0.120000 stress 0.012752 penalty 0.234937
## itel    1 lambda   0.130000 stress 0.014677 penalty 0.224281
## itel    1 lambda   0.140000 stress 0.016766 penalty 0.213553
## itel    1 lambda   0.150000 stress 0.019004 penalty 0.202867
## itel    1 lambda   0.160000 stress 0.021375 penalty 0.192317
## itel    1 lambda   0.170000 stress 0.023863 penalty 0.181981
## itel    1 lambda   0.180000 stress 0.026446 penalty 0.171921
## itel    1 lambda   0.190000 stress 0.029107 penalty 0.162184
## itel    1 lambda   0.200000 stress 0.031826 penalty 0.152804
## itel    1 lambda   0.210000 stress 0.034585 penalty 0.143802
## itel    1 lambda   0.220000 stress 0.037368 penalty 0.135189
## itel    1 lambda   0.230000 stress 0.040161 penalty 0.126967
## itel    1 lambda   0.240000 stress 0.042951 penalty 0.119133
## itel    1 lambda   0.250000 stress 0.045728 penalty 0.111680
## itel    1 lambda   0.260000 stress 0.048483 penalty 0.104597
## itel    1 lambda   0.270000 stress 0.051208 penalty 0.097873
## itel    1 lambda   0.280000 stress 0.053896 penalty 0.091496
## itel    1 lambda   0.290000 stress 0.056540 penalty 0.085455
## itel    1 lambda   0.300000 stress 0.059136 penalty 0.079739
## itel    1 lambda   0.310000 stress 0.061677 penalty 0.074338
## itel    1 lambda   0.320000 stress 0.064160 penalty 0.069241
## itel    1 lambda   0.330000 stress 0.066580 penalty 0.064438
## itel    1 lambda   0.340000 stress 0.068935 penalty 0.059918
## itel    1 lambda   0.350000 stress 0.071222 penalty 0.055668
## itel    1 lambda   0.700000 stress 0.109679 penalty 0.000427
## itel    1 lambda   0.710000 stress 0.109756 penalty 0.000320
## itel   92 lambda   0.720000 stress 0.109880 penalty 0.000000
```



Intelligence

These are correlations between eight intelligence tests, taken from the `smacof` package. We convert to dissimilarities by taking the negative logarithm of the correlations.

Using the Torgerson initial configuration in two dimensions, smacof finds a stress of 0.0075160651 after 28 iterations. This corresponds with the presumed global minimum.

A full-dimensional scaling with $p = 7$ gives stress 0.0049386956 after 1554 iterations. The singular values of the full dimensional solution are

```
## [1] +0.382699 +0.291593 +0.127580 +0.031521 +0.003190 +0.000000 +0.000000
```

and thus the Gower rank of these data is five.

If we our smacof iterations with the first two dimensions of the full dimensional solution stress is 0.0075160651 after 26 iterations, the same solution as with the Torgerson start.

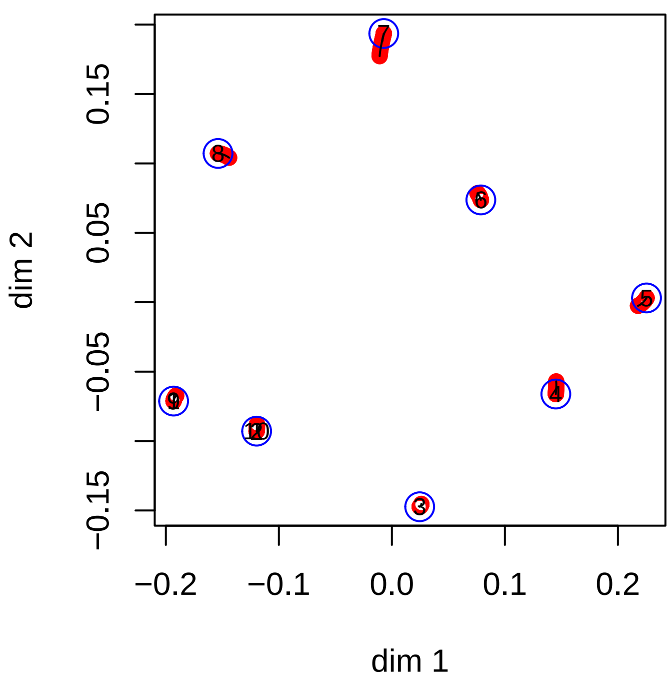
If we run smacof 1000 times with a random start we find two different local minima, and the one with the smallest stress is found in about 90% of the cases. Again, this is the same solution.

```
##
## 0.163122  1.24546
##       896      104
```

Our global optimization method with the default λ sequence also converges to the same solution.

```
## itel 1553 lambda   0.000000 stress 0.004939 penalty 0.368081
## itel    7 lambda   0.010000 stress 0.004956 penalty 0.031597
```

```
## itel    4 lambda   0.020000 stress 0.005001 penalty 0.028964
## itel    3 lambda   0.030000 stress 0.005070 penalty 0.026414
## itel    3 lambda   0.040000 stress 0.005181 penalty 0.023535
## itel    2 lambda   0.050000 stress 0.005286 penalty 0.021411
## itel    2 lambda   0.060000 stress 0.005420 penalty 0.019125
## itel    2 lambda   0.070000 stress 0.005580 penalty 0.016798
## itel    2 lambda   0.080000 stress 0.005760 penalty 0.014516
## itel    2 lambda   0.090000 stress 0.005954 penalty 0.012341
## itel    2 lambda   0.100000 stress 0.006155 penalty 0.010317
## itel    2 lambda   0.110000 stress 0.006356 penalty 0.008472
## itel    3 lambda   0.120000 stress 0.006631 penalty 0.006162
## itel    2 lambda   0.130000 stress 0.006795 penalty 0.004892
## itel    4 lambda   0.140000 stress 0.007060 penalty 0.002972
## itel    4 lambda   0.150000 stress 0.007241 penalty 0.001739
## itel    9 lambda   0.160000 stress 0.007438 penalty 0.000476
## itel   52 lambda   0.170000 stress 0.007516 penalty 0.000000
## itel    8 lambda   0.180000 stress 0.007516 penalty 0.000000
## itel    4 lambda   0.190000 stress 0.007516 penalty 0.000000
## itel    2 lambda   0.200000 stress 0.007516 penalty 0.000000
## itel    2 lambda   0.210000 stress 0.007516 penalty 0.000000
```



As in the chi-square example, the FDS and the 2MDS solution are very similar and the PMDS trajectories are short.

Countries

This is the `wish` dataset from the 'smacof' package, with similarities between 12 countries. They are converted to dissimilarties by subtracting each of them from seven.

```
data(wish, package = "smacof")
countries <- as.matrix(wish)
w <- matrix(1, 12, 12) - diag(12)
countries <- 7 * w - countries
countries <- 2 * countries / sqrt(sum(w * countries * countries))
```

Using the Torgerson initial configuration in two dimensions, smacof finds a stress of 0.0477490806 after 103 iterations.

A full-dimensional scaling with $p = 11$ gives stress 0.0159699675 after 763 iterations. The singular values of the full dimensional solution are

```
##  [1] +0.256524 +0.226618 +0.163113 +0.109658 +0.081072 +0.040506 +0.000595
##  [8] +0.000000 +0.000000 +0.000000 +0.000000
```

and thus the Gower rank of these data is seven.

If we start our smacof iterations with the first two dimensions of the full dimensional solution then stress is 0.0477490807 after 95 iterations, and we find the same solution as with the Torgerson start.

If we run smacof 1000 times with a random start we find sixteen different local minima, and the one with the smallest stress is found in about 35% of the cases. Note, however, that the Torgerson and full-dimensional solutions correspond with the second smallest local minimum, which is consequently certainly not the global minimum.

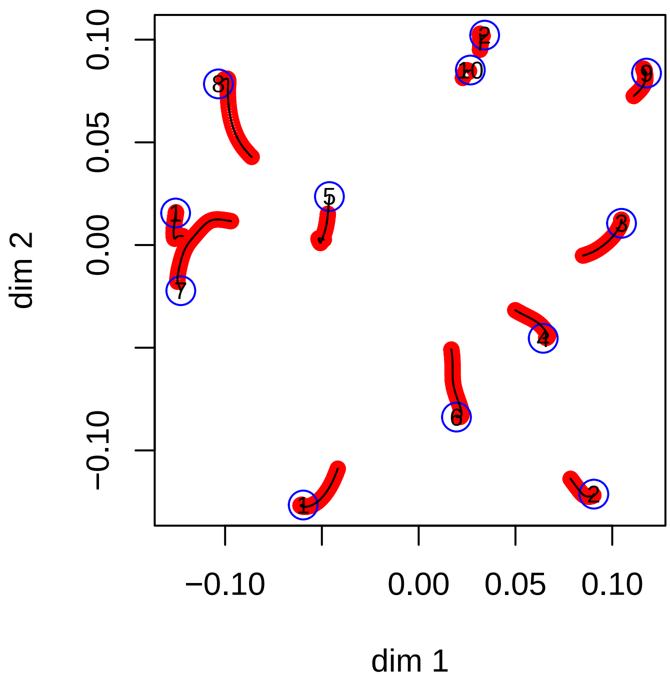
```
##
## 0.0474139 0.0477491 0.0494938 0.0513037 0.0669776 0.0671137 0.0691977 0.0698188
##       357       185       138       104        55        60        35        29
## 0.0898758 0.0909081 0.0913887 0.0914608 0.0917437  0.100849  0.102294  0.107119
##         4         7         4         5         3         6         7         1
```

Our global optimization method with the default λ sequence does converge to the solution with minimum stress 0.0474139053, which is our tentative global minimum.

```
## itel  802 lambda   0.000000 stress 0.015970 penalty 0.367070
## itel    4 lambda   0.010000 stress 0.016010 penalty 0.134507
## itel    3 lambda   0.020000 stress 0.016140 penalty 0.128004
## itel    2 lambda   0.030000 stress 0.016331 penalty 0.122297
## itel    1 lambda   0.040000 stress 0.016515 penalty 0.118330
## itel    1 lambda   0.050000 stress 0.016780 penalty 0.113631
## itel    1 lambda   0.060000 stress 0.017127 penalty 0.108490
## itel    1 lambda   0.070000 stress 0.017557 penalty 0.103107
## itel    1 lambda   0.080000 stress 0.018068 penalty 0.097622
## itel    1 lambda   0.090000 stress 0.018654 penalty 0.092138
```

```
## itel    1 lambda   0.100000 stress 0.019310 penalty 0.086729
## itel    1 lambda   0.110000 stress 0.020028 penalty 0.081447
## itel    1 lambda   0.120000 stress 0.020801 penalty 0.076329
## itel    1 lambda   0.130000 stress 0.021620 penalty 0.071403
## itel    1 lambda   0.140000 stress 0.022479 penalty 0.066685
## itel    1 lambda   0.150000 stress 0.023369 penalty 0.062184
## itel    1 lambda   0.160000 stress 0.024283 penalty 0.057904
## itel    1 lambda   0.170000 stress 0.025215 penalty 0.053847
## itel    1 lambda   0.180000 stress 0.026159 penalty 0.050009
## itel    1 lambda   0.190000 stress 0.027110 penalty 0.046385
## itel    1 lambda   0.200000 stress 0.028062 penalty 0.042967
## itel    1 lambda   0.210000 stress 0.029011 penalty 0.039749
## itel    1 lambda   0.220000 stress 0.029953 penalty 0.036722
## itel    1 lambda   0.230000 stress 0.030885 penalty 0.033877
## itel    1 lambda   0.240000 stress 0.031802 penalty 0.031208
## itel    1 lambda   0.250000 stress 0.032702 penalty 0.028706
## itel    1 lambda   0.260000 stress 0.033582 penalty 0.026364
## itel    1 lambda   0.270000 stress 0.034440 penalty 0.024176
## itel    1 lambda   0.280000 stress 0.035273 penalty 0.022136
## itel    1 lambda   0.290000 stress 0.036079 penalty 0.020237
## itel    1 lambda   0.300000 stress 0.036857 penalty 0.018474
## itel    1 lambda   0.310000 stress 0.037604 penalty 0.016841
## itel    1 lambda   0.320000 stress 0.038319 penalty 0.015332
## itel    1 lambda   0.330000 stress 0.039003 penalty 0.013940
## itel    1 lambda   0.340000 stress 0.039654 penalty 0.012659
## itel    1 lambda   0.350000 stress 0.040272 penalty 0.011482
## itel    1 lambda   0.360000 stress 0.040858 penalty 0.010403
## itel    1 lambda   0.370000 stress 0.041413 penalty 0.009413
## itel    1 lambda   0.380000 stress 0.041936 penalty 0.008508
## itel    1 lambda   0.390000 stress 0.042428 penalty 0.007679
## itel    1 lambda   0.400000 stress 0.042892 penalty 0.006922
## itel    1 lambda   0.410000 stress 0.043326 penalty 0.006229
## itel    1 lambda   0.420000 stress 0.043734 penalty 0.005595
## itel    1 lambda   0.430000 stress 0.044116 penalty 0.005015
## itel    1 lambda   0.440000 stress 0.044472 penalty 0.004483
## itel    1 lambda   0.450000 stress 0.044803 penalty 0.003995
## itel    1 lambda   0.460000 stress 0.045112 penalty 0.003547
## itel    1 lambda   0.470000 stress 0.045397 penalty 0.003133
## itel    1 lambda   0.480000 stress 0.045660 penalty 0.002751
## itel    1 lambda   0.490000 stress 0.045902 penalty 0.002398
## itel    1 lambda   0.500000 stress 0.046124 penalty 0.002071
## itel    1 lambda   0.510000 stress 0.046325 penalty 0.001769
## itel    1 lambda   0.520000 stress 0.046506 penalty 0.001492
## itel    1 lambda   0.530000 stress 0.046668 penalty 0.001240
## itel    1 lambda   0.540000 stress 0.046811 penalty 0.001016
```

```
## itel    1 lambda   0.550000 stress 0.046934 penalty 0.000819
## itel    1 lambda   0.560000 stress 0.047040 penalty 0.000651
## itel    1 lambda   0.570000 stress 0.047128 penalty 0.000509
## itel    1 lambda   0.580000 stress 0.047200 penalty 0.000392
## itel    1 lambda   0.590000 stress 0.047258 penalty 0.000298
## itel    1 lambda   0.600000 stress 0.047303 penalty 0.000224
## itel   68 lambda   0.610000 stress 0.047414 penalty 0.000000
```



Dutch Political Parties

In 1967 one hundred psychology students at Leiden University judged the similarity of nine Dutch political parties, using the complete method of triads (De Gruijter (1967)). Data were aggregated and converted to dissimilarities. We first print the matrix of dissimilarities.

```
##        KVP    PvdA   VVD    ARP    CHU    CPN    PSP    BP     D66
## KVP  +0.000 +0.209 +0.196 +0.171 +0.179 +0.281 +0.250 +0.267 +0.230
## PvdA +0.209 +0.000 +0.250 +0.210 +0.231 +0.190 +0.171 +0.269 +0.204
## VVD  +0.196 +0.250 +0.000 +0.203 +0.185 +0.302 +0.281 +0.257 +0.174
## ARP  +0.171 +0.210 +0.203 +0.000 +0.119 +0.292 +0.250 +0.271 +0.228
## CHU  +0.179 +0.231 +0.185 +0.119 +0.000 +0.290 +0.263 +0.259 +0.225
## CPN  +0.281 +0.190 +0.302 +0.292 +0.290 +0.000 +0.152 +0.236 +0.276
## PSP  +0.250 +0.171 +0.281 +0.250 +0.263 +0.152 +0.000 +0.256 +0.237
## BP   +0.267 +0.269 +0.257 +0.271 +0.259 +0.236 +0.256 +0.000 +0.274
## D66  +0.230 +0.204 +0.174 +0.228 +0.225 +0.276 +0.237 +0.274 +0.000
```

```
##        KVP    PvdA   VVD    ARP    CHU    CPN    PSP    BP     D66
## KVP  +0.000 +0.128 +0.099 +0.054 +0.066 +0.348 +0.242 +0.299 +0.179
## PvdA +0.128 +0.000 +0.241 +0.129 +0.185 +0.088 +0.054 +0.304 +0.115
```

```
## VVD  +0.099 +0.241 +0.000 +0.114 +0.077 +0.438 +0.350 +0.263 +0.058
## ARP  +0.054 +0.129 +0.114 +0.000 +0.004 +0.393 +0.242 +0.312 +0.175
## CHU  +0.066 +0.185 +0.077 +0.004 +0.000 +0.387 +0.286 +0.270 +0.166
## CPN  +0.348 +0.088 +0.438 +0.393 +0.387 +0.000 +0.029 +0.197 +0.331
## PSP  +0.242 +0.054 +0.350 +0.242 +0.286 +0.029 +0.000 +0.260 +0.200
## BP   +0.299 +0.304 +0.263 +0.312 +0.270 +0.197 +0.260 +0.000 +0.323
## D66  +0.179 +0.115 +0.058 +0.175 +0.166 +0.331 +0.200 +0.323 +0.000
```

This is mainly because these data, being averages over a heterogeneous group of individuals, regress to the mean and thus have a substantial additive constant.

Using the Torgerson initial configuration in two dimensions, smacof finds a stress of 0.0272187083 after 97 iterations.

A full-dimensional scaling with $p = 8$ gives stress 0.0218562551 after 68 iterations. The singular values of the full dimensional solution are

```
## [1] +0.389414 +0.216045 +0.132915 +0.037145 +0.000000 +0.000000 +0.000000
## [8] +0.000000
```

and thus the Gower rank of these (transformed) data is four.

If we start our smacof iterations with the first two dimensions of the full dimensional solution stress is 0.0272187083 after 78 iterations, the same solution as with the Torgerson start.

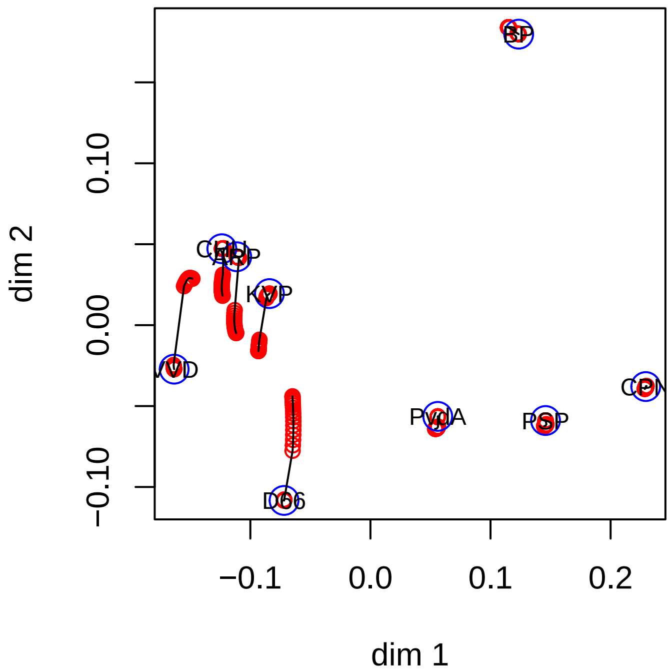
If we run smacof 1000 times with a random start we find two different local minima, and the one with the smallest stress is found in about 55% of the cases.

```
##
## 0.0272187 0.0301047
##       566       434
```

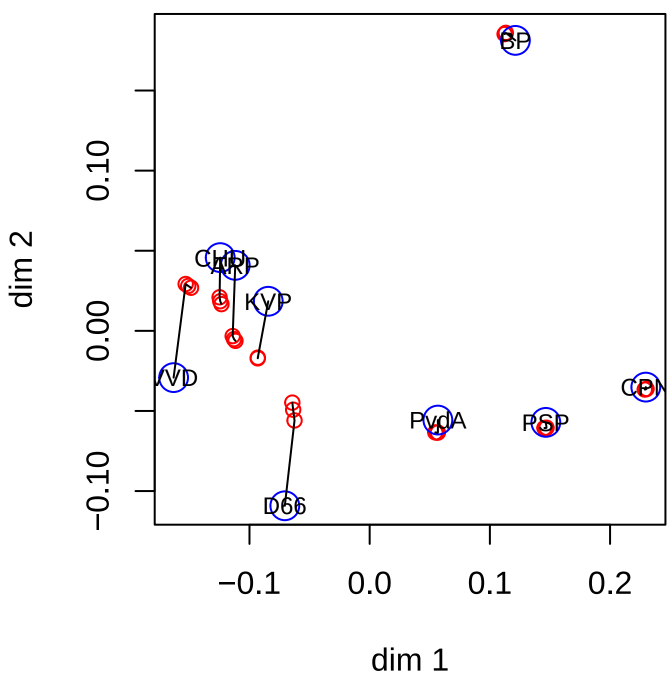
Our global optimization method with the default λ sequence also converges to the same smallest local minimum.

```
## itel   80 lambda   0.000000 stress 0.021856 penalty 0.453217
## itel    2 lambda   0.010000 stress 0.021865 penalty 0.041599
## itel    2 lambda   0.020000 stress 0.021899 penalty 0.040014
## itel    1 lambda   0.030000 stress 0.021938 penalty 0.038919
## itel    1 lambda   0.040000 stress 0.022002 penalty 0.037599
## itel    1 lambda   0.050000 stress 0.022091 penalty 0.036178
## itel    1 lambda   0.060000 stress 0.022205 penalty 0.034717
## itel    1 lambda   0.070000 stress 0.022342 penalty 0.033247
## itel    1 lambda   0.080000 stress 0.022499 penalty 0.031782
## itel    1 lambda   0.090000 stress 0.022675 penalty 0.030330
## itel    1 lambda   0.100000 stress 0.022868 penalty 0.028890
## itel    1 lambda   0.110000 stress 0.023077 penalty 0.027462
## itel    1 lambda   0.120000 stress 0.023299 penalty 0.026041
## itel    1 lambda   0.130000 stress 0.023532 penalty 0.024623
## itel    1 lambda   0.140000 stress 0.023776 penalty 0.023204
```

```
## itel    1 lambda   0.150000 stress 0.024028 penalty 0.021779
## itel    1 lambda   0.160000 stress 0.024286 penalty 0.020344
## itel    1 lambda   0.170000 stress 0.024548 penalty 0.018899
## itel    1 lambda   0.180000 stress 0.024811 penalty 0.017442
## itel   31 lambda   0.190000 stress 0.026907 penalty 0.001050
## itel    1 lambda   0.200000 stress 0.026926 penalty 0.000956
## itel    1 lambda   0.210000 stress 0.026948 penalty 0.000864
## itel    1 lambda   0.220000 stress 0.026971 penalty 0.000773
## itel    1 lambda   0.230000 stress 0.026995 penalty 0.000685
## itel    1 lambda   0.240000 stress 0.027018 penalty 0.000600
## itel    1 lambda   0.250000 stress 0.027042 penalty 0.000521
## itel    1 lambda   0.260000 stress 0.027064 penalty 0.000448
## itel    1 lambda   0.270000 stress 0.027084 penalty 0.000382
## itel    1 lambda   0.280000 stress 0.027104 penalty 0.000322
## itel    1 lambda   0.290000 stress 0.027121 penalty 0.000269
## itel    1 lambda   0.300000 stress 0.027137 penalty 0.000222
## itel    1 lambda   0.310000 stress 0.027152 penalty 0.000181
## itel    1 lambda   0.320000 stress 0.027164 penalty 0.000147
## itel    1 lambda   0.330000 stress 0.027175 penalty 0.000117
## itel    1 lambda   0.340000 stress 0.027184 penalty 0.000092
## itel    1 lambda   0.350000 stress 0.027191 penalty 0.000072
## itel    1 lambda   0.360000 stress 0.027197 penalty 0.000055
## itel    1 lambda   0.370000 stress 0.027202 penalty 0.000042
## itel    1 lambda   0.380000 stress 0.027206 penalty 0.000032
## itel    6 lambda   0.390000 stress 0.027217 penalty 0.000005
## itel   18 lambda   0.400000 stress 0.027219 penalty 0.000000
## itel    2 lambda   0.410000 stress 0.027219 penalty 0.000000
## itel    2 lambda   0.420000 stress 0.027219 penalty 0.000000
```




```
## itel   80 lambda   0.000000 stress 0.021856 penalty 0.453217
## itel    3 lambda   0.111111 stress 0.022908 penalty 0.029330
## itel    2 lambda   0.222222 stress 0.024912 penalty 0.020271
## itel   71 lambda   0.333333 stress 0.027219 penalty 0.000000
```



Ekman

The next example analyzes dissimilarities between 14 colors, taken from Ekman (1954). The original similarities s_{ij}, averaged over 31 subjects, were transformed to dissimilarities by

$\delta_{ij} = 1 - s_{ij}$.

Using the Torgerson initial configuration in two dimensions, smacof finds a stress of 0.0172132469 after 25 iterations.

A full-dimensional scaling with $p = 8$ gives stress $8.7569296565 \times 10^{-5}$ after 1204 iterations. The singular values of the full dimensional solution are

```
##  [1] +0.254220 +0.205722 +0.119338 +0.109900 +0.068741 +0.055643 +0.033137
##  [8] +0.022797 +0.011573 +0.001704 +0.000315 +0.000000 +0.000000
```

and thus the Gower rank of these (transformed) data is eleven.

If we start our smacof iterations with the first two dimensions of the full dimensional solution stress is 0.0172132469 after 25 iterations, the same solution as with the Torgerson start.

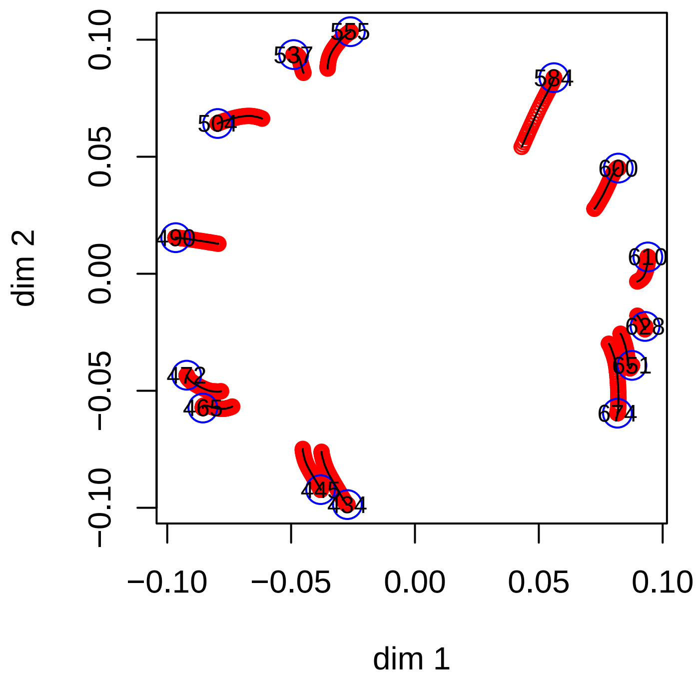
If we run smacof 1000 times with a random start we find ten different local minima, and the one with the smallest stress is found in about 80% of the cases.

```
##
## 0.0172132 0.0365429 0.0601969 0.0619843  0.063479 0.0662027 0.0674562 0.0678714
##       834       133        15         6         3         3         2         2
## 0.0758563 0.0759964
##         1         1
```

Our global optimization method with the default λ sequence also converges to the same smallest local minimum.

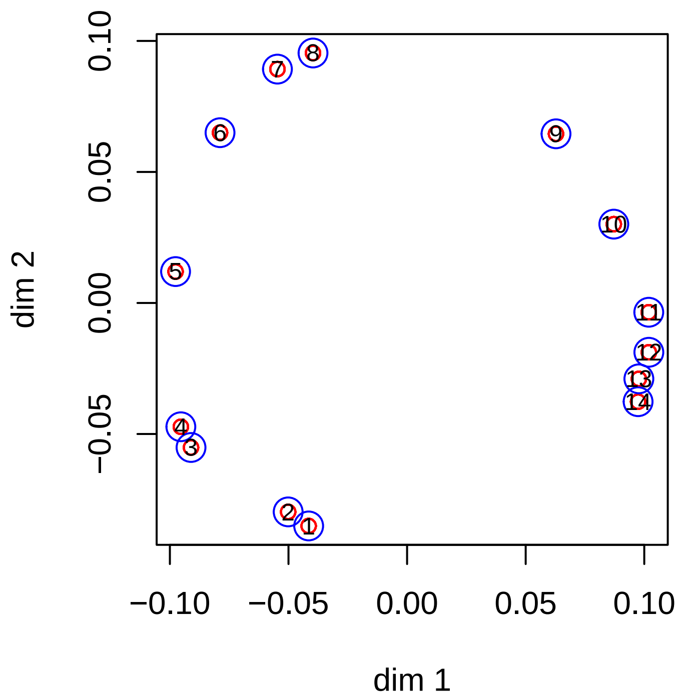
```
## itel 1482 lambda   0.000000 stress 0.000088 penalty 0.426110
## itel    5 lambda   0.010000 stress 0.000132 penalty 0.118988
## itel    3 lambda   0.020000 stress 0.000253 penalty 0.112777
## itel    2 lambda   0.030000 stress 0.000431 penalty 0.107184
## itel    2 lambda   0.040000 stress 0.000715 penalty 0.100691
## itel    1 lambda   0.050000 stress 0.000942 penalty 0.096656
## itel    1 lambda   0.060000 stress 0.001246 penalty 0.091999
## itel    1 lambda   0.070000 stress 0.001627 penalty 0.086941
## itel    1 lambda   0.080000 stress 0.002082 penalty 0.081645
## itel    1 lambda   0.090000 stress 0.002607 penalty 0.076232
## itel    1 lambda   0.100000 stress 0.003195 penalty 0.070791
## itel    1 lambda   0.110000 stress 0.003840 penalty 0.065388
## itel    1 lambda   0.120000 stress 0.004534 penalty 0.060073
## itel    1 lambda   0.130000 stress 0.005267 penalty 0.054886
## itel    1 lambda   0.140000 stress 0.006033 penalty 0.049859
## itel    1 lambda   0.150000 stress 0.006820 penalty 0.045021
## itel    1 lambda   0.160000 stress 0.007622 penalty 0.040395
## itel    1 lambda   0.170000 stress 0.008427 penalty 0.036003
## itel    1 lambda   0.180000 stress 0.009228 penalty 0.031864
## itel    1 lambda   0.190000 stress 0.010014 penalty 0.027995
## itel    1 lambda   0.200000 stress 0.010778 penalty 0.024407
```

```
## itel    1 lambda   0.210000 stress 0.011510 penalty 0.021111
## itel    1 lambda   0.220000 stress 0.012203 penalty 0.018110
## itel    1 lambda   0.230000 stress 0.012852 penalty 0.015406
## itel    1 lambda   0.240000 stress 0.013451 penalty 0.012993
## itel    1 lambda   0.250000 stress 0.013997 penalty 0.010863
## itel    1 lambda   0.260000 stress 0.014489 penalty 0.009003
## itel    1 lambda   0.270000 stress 0.014926 penalty 0.007396
## itel    2 lambda   0.280000 stress 0.015618 penalty 0.004939
## itel    1 lambda   0.290000 stress 0.015890 penalty 0.004012
## itel    1 lambda   0.300000 stress 0.016125 penalty 0.003230
## itel    2 lambda   0.310000 stress 0.016484 penalty 0.002072
## itel    1 lambda   0.320000 stress 0.016620 penalty 0.001651
## itel    1 lambda   0.330000 stress 0.016734 penalty 0.001305
## itel    2 lambda   0.340000 stress 0.016904 penalty 0.000807
## itel    1 lambda   0.350000 stress 0.016966 penalty 0.000632
## itel    1 lambda   0.360000 stress 0.017017 penalty 0.000491
## itel    1 lambda   0.370000 stress 0.017059 penalty 0.000378
## itel    1 lambda   0.380000 stress 0.017093 penalty 0.000289
## itel    1 lambda   0.390000 stress 0.017121 penalty 0.000219
## itel    1 lambda   0.400000 stress 0.017142 penalty 0.000165
## itel    2 lambda   0.410000 stress 0.017172 penalty 0.000092
## itel    1 lambda   0.420000 stress 0.017183 penalty 0.000068
## itel    1 lambda   0.430000 stress 0.017190 penalty 0.000050
## itel    1 lambda   0.440000 stress 0.017196 penalty 0.000037
## itel    2 lambda   0.450000 stress 0.017204 penalty 0.000019
## itel    2 lambda   0.460000 stress 0.017209 penalty 0.000010
## itel    2 lambda   0.470000 stress 0.017211 penalty 0.000005
## itel    3 lambda   0.480000 stress 0.017212 penalty 0.000002
## itel    4 lambda   0.490000 stress 0.017213 penalty 0.000000
## itel    4 lambda   0.500000 stress 0.017213 penalty 0.000000
## itel    4 lambda   0.510000 stress 0.017213 penalty 0.000000
## itel    2 lambda   0.520000 stress 0.017213 penalty 0.000000
```



If we transform the Ekman similarities by $\delta_{ij} = (1 - s_{ij})^3$ then it is known (De Leeuw (2016)) that the Gower rank of the transformed data is equal to two. Thus the FDS solution has rank 2, and the 2MDS solution always the global minimum.

```
## itel   99 lambda   0.000000 stress 0.011025 penalty 0.433456
## itel    1 lambda   0.010000 stress 0.011025 penalty 0.000000
## itel    1 lambda   0.020000 stress 0.011025 penalty 0.000000
## itel    1 lambda   0.030000 stress 0.011025 penalty 0.000000
## itel    1 lambda   0.040000 stress 0.011025 penalty 0.000000
## itel    1 lambda   0.050000 stress 0.011025 penalty 0.000000
## itel    1 lambda   0.060000 stress 0.011025 penalty 0.000000
## itel    1 lambda   0.070000 stress 0.011025 penalty 0.000000
## itel    1 lambda   0.080000 stress 0.011025 penalty 0.000000
## itel    1 lambda   0.090000 stress 0.011025 penalty 0.000000
## itel    1 lambda   0.100000 stress 0.011025 penalty 0.000000
## itel    1 lambda   0.110000 stress 0.011025 penalty 0.000000
## itel    1 lambda   0.120000 stress 0.011025 penalty 0.000000
## itel    1 lambda   0.130000 stress 0.011025 penalty 0.000000
```



Morse in Two

Next, we use dissimilarities between 36 Morse code signals (Rothkopf (1957)). We used the symmetrized version `morse` from the `smacof` package (De Leeuw and Mair (2009)).

Using the Torgerson initial configuration in two dimensions, smacof finds a stress of 0.0899492031 after 238 iterations.

A full-dimensional scaling with $p = 31$ gives stress $7.6345177128 \times 10^{-4}$ after 1347 iterations. The singular values of the full dimensional solution are

```
##  [1] +0.100442 +0.090156 +0.078222 +0.067738 +0.061768 +0.060456 +0.055417
##  [8] +0.049762 +0.047491 +0.045725 +0.044117 +0.039553 +0.036242 +0.033715
## [15] +0.032183 +0.025291 +0.022152 +0.019617 +0.018309 +0.013419 +0.012242
## [22] +0.006957 +0.000575 +0.000071 +0.000014 +0.000000 +0.000000 +0.000000
## [29] +0.000000 +0.000000 +0.000000 +0.000000 +0.000000 +0.000000 +0.000000
```

and thus the Gower rank of these (transformed) data is 25.

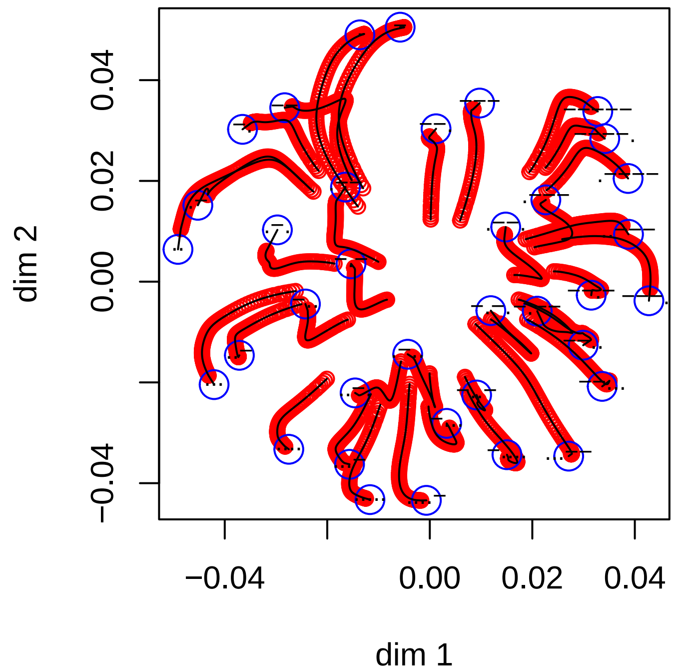
If we start our smacof iterations with the first two dimensions of the full dimensional solution stress is 0.0899492031 after 238 iterations, the same solution as with the Torgerson start.

If we run smacof 1000 times with a random start we find a huge number of local minima. It is difficult to draw the line on which local minima are the same and which are different, but our usual procedure says there are 684 of them. It would be silly to print them out here. Suffices it to say that the smallest stress is 0.0899492025, which is found in only about 7% of the cases. It is the same as stress for the previous Torgerson and FDS solutions.

Our global optimization method with the default λ sequence also converges to the same smallest local minimum.

```
## itel 1461 lambda   0.000000 stress 0.000763 penalty 0.472254
## itel    6 lambda   0.010000 stress 0.000858 penalty 0.322181
## itel    4 lambda   0.020000 stress 0.001147 penalty 0.308335
## itel    3 lambda   0.030000 stress 0.001622 penalty 0.294777
## itel    2 lambda   0.040000 stress 0.002207 penalty 0.283003
## itel    2 lambda   0.050000 stress 0.003018 penalty 0.269965
## itel    1 lambda   0.060000 stress 0.003720 penalty 0.261134
## itel    2 lambda   0.070000 stress 0.005058 penalty 0.245658
## itel    1 lambda   0.080000 stress 0.006058 penalty 0.236320
## itel    1 lambda   0.090000 stress 0.007232 penalty 0.226392
## itel    1 lambda   0.100000 stress 0.008576 penalty 0.216089
## itel    1 lambda   0.110000 stress 0.010085 penalty 0.205587
## itel    1 lambda   0.120000 stress 0.011750 penalty 0.195030
## itel    1 lambda   0.130000 stress 0.013559 penalty 0.184543
## itel    1 lambda   0.140000 stress 0.015500 penalty 0.174225
## itel    1 lambda   0.150000 stress 0.017554 penalty 0.164160
## itel    1 lambda   0.160000 stress 0.019705 penalty 0.154411
## itel    1 lambda   0.170000 stress 0.021934 penalty 0.145029
## itel    1 lambda   0.180000 stress 0.024222 penalty 0.136047
## itel    1 lambda   0.190000 stress 0.026550 penalty 0.127488
## itel    1 lambda   0.200000 stress 0.028903 penalty 0.119364
## itel    1 lambda   0.210000 stress 0.031265 penalty 0.111677
## itel    1 lambda   0.220000 stress 0.033621 penalty 0.104423
## itel    1 lambda   0.230000 stress 0.035962 penalty 0.097591
## itel    1 lambda   0.240000 stress 0.038277 penalty 0.091167
## itel    1 lambda   0.250000 stress 0.040558 penalty 0.085132
## itel    1 lambda   0.260000 stress 0.042799 penalty 0.079467
## itel    1 lambda   0.270000 stress 0.044995 penalty 0.074148
## itel    1 lambda   0.280000 stress 0.047143 penalty 0.069155
## itel    1 lambda   0.290000 stress 0.049240 penalty 0.064466
## itel    1 lambda   0.300000 stress 0.051285 penalty 0.060060
## itel    1 lambda   0.310000 stress 0.053275 penalty 0.055920
## itel    1 lambda   0.320000 stress 0.055211 penalty 0.052027
## itel    1 lambda   0.330000 stress 0.057092 penalty 0.048366
## itel    1 lambda   0.340000 stress 0.058916 penalty 0.044923
## itel    1 lambda   0.350000 stress 0.060683 penalty 0.041685
## itel    1 lambda   0.360000 stress 0.062393 penalty 0.038640
## itel    1 lambda   0.370000 stress 0.064045 penalty 0.035778
## itel    1 lambda   0.380000 stress 0.065639 penalty 0.033088
## itel    1 lambda   0.390000 stress 0.067175 penalty 0.030562
## itel    1 lambda   0.400000 stress 0.068653 penalty 0.028190
## itel    1 lambda   0.410000 stress 0.070072 penalty 0.025963
## itel    1 lambda   0.420000 stress 0.071433 penalty 0.023875
```

```
## itel    1 lambda   0.430000 stress 0.072735 penalty 0.021917
## itel    1 lambda   0.440000 stress 0.073980 penalty 0.020083
## itel    1 lambda   0.450000 stress 0.075168 penalty 0.018366
## itel    1 lambda   0.460000 stress 0.076298 penalty 0.016761
## itel    1 lambda   0.470000 stress 0.077371 penalty 0.015263
## itel    1 lambda   0.480000 stress 0.078389 penalty 0.013865
## itel    1 lambda   0.490000 stress 0.079351 penalty 0.012564
## itel    1 lambda   0.500000 stress 0.080258 penalty 0.011356
## itel    1 lambda   0.510000 stress 0.081112 penalty 0.010237
## itel    1 lambda   0.520000 stress 0.081912 penalty 0.009204
## itel    1 lambda   0.530000 stress 0.082661 penalty 0.008252
## itel    1 lambda   0.540000 stress 0.083360 penalty 0.007379
## itel    1 lambda   0.550000 stress 0.084009 penalty 0.006580
## itel    1 lambda   0.560000 stress 0.084610 penalty 0.005853
## itel    1 lambda   0.570000 stress 0.085165 penalty 0.005194
## itel    1 lambda   0.580000 stress 0.085676 penalty 0.004598
## itel    1 lambda   0.590000 stress 0.086144 penalty 0.004061
## itel    1 lambda   0.600000 stress 0.086572 penalty 0.003578
## itel    1 lambda   0.610000 stress 0.086962 penalty 0.003145
## itel    1 lambda   0.620000 stress 0.087316 penalty 0.002757
## itel    1 lambda   0.630000 stress 0.087637 penalty 0.002411
## itel    1 lambda   0.640000 stress 0.087927 penalty 0.002102
## itel    1 lambda   0.650000 stress 0.088188 penalty 0.001827
## itel    1 lambda   0.660000 stress 0.088423 penalty 0.001582
## itel    1 lambda   0.670000 stress 0.088633 penalty 0.001365
## itel    1 lambda   0.680000 stress 0.088822 penalty 0.001173
## itel    1 lambda   0.690000 stress 0.088990 penalty 0.001003
## itel    1 lambda   0.700000 stress 0.089140 penalty 0.000854
## itel    1 lambda   0.710000 stress 0.089273 penalty 0.000723
## itel    1 lambda   0.720000 stress 0.089390 penalty 0.000608
## itel    1 lambda   0.730000 stress 0.089493 penalty 0.000509
## itel    1 lambda   0.740000 stress 0.089583 penalty 0.000422
## itel    1 lambda   0.750000 stress 0.089660 penalty 0.000348
## itel    1 lambda   0.760000 stress 0.089726 penalty 0.000284
## itel    1 lambda   0.770000 stress 0.089782 penalty 0.000230
## itel    1 lambda   0.780000 stress 0.089828 penalty 0.000185
## itel    1 lambda   0.790000 stress 0.089867 penalty 0.000147
## itel    1 lambda   0.800000 stress 0.089898 penalty 0.000116
## itel    1 lambda   0.810000 stress 0.089923 penalty 0.000090
## itel    1 lambda   0.820000 stress 0.089943 penalty 0.000070
## itel    1 lambda   0.830000 stress 0.089958 penalty 0.000053
## itel    1 lambda   0.840000 stress 0.089970 penalty 0.000040
## itel  197 lambda   0.850000 stress 0.089949 penalty 0.000000
```



Vegetables

Our first one-dimensional example uses paired comparisons of 9 vegetables, originating with Guilford (1954) and taken from the `psychTools` package (Revelle (2023)). The proportions are transformed to dissimilarities by using the normal quantile function, i.e. $\delta_{ij} = |\Phi^{-1}(p_{ij})|$.

Using the Torgerson initial configuration in two dimensions, smacof finds a stress of 0.0353011713 after 3 iterations.

A full-dimensional scaling with $p = 8$ gives stress 0.0136747248 after 1378 iterations. The singular values of the full dimensional solution are

```
## [1] +0.406637 +0.209179 +0.100334 +0.002692 +0.000000 +0.000000 +0.000000
## [8] +0.000000
```

and thus the Gower rank of these (transformed) data is 4.

If we start our smacof iterations with the first dimension of the full dimensional solution stress is 0.0353011713 after 3 iterations, the same solution as with the Torgerson start.

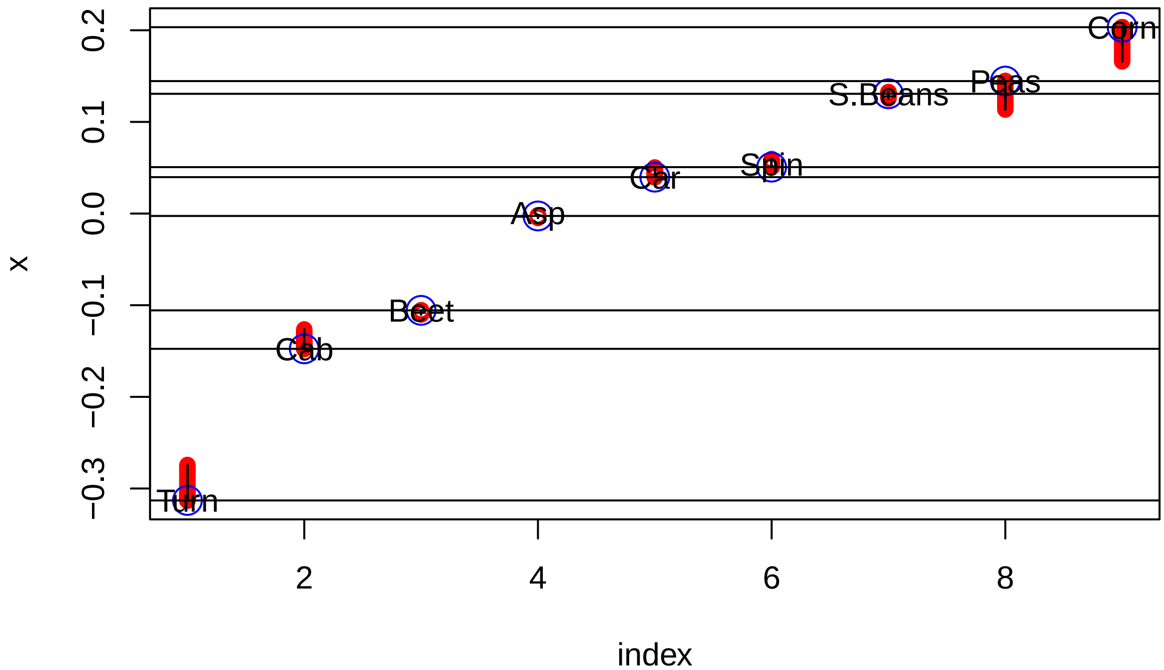
If we run smacof 1000 times with a random start we find a huge number of local minima. It is difficult to draw the line on which local minima are the same and which are different, but our usual procedure says there are 665 of them. It would be silly to print them all out here. Suffices it to say that the smallest stress is 0.0353011713, which is found in only about 10% of the cases. It is the same as stress for the previous Torgerson and FDS solutions.

Our global optimization method with the default λ sequence also converges to the same smallest local minimum.

```
## itel 1412 lambda   0.000000 stress 0.013675 penalty 0.269308
```

```
## itel    5 lambda   0.010000 stress 0.013716 penalty 0.114786
## itel    3 lambda   0.020000 stress 0.013831 penalty 0.108848
## itel    2 lambda   0.030000 stress 0.014001 penalty 0.103509
## itel    2 lambda   0.040000 stress 0.014271 penalty 0.097345
## itel    1 lambda   0.050000 stress 0.014489 penalty 0.093513
## itel    1 lambda   0.060000 stress 0.014782 penalty 0.089107
## itel    1 lambda   0.070000 stress 0.015148 penalty 0.084346
## itel    1 lambda   0.080000 stress 0.015587 penalty 0.079388
## itel    1 lambda   0.090000 stress 0.016095 penalty 0.074352
## itel    1 lambda   0.100000 stress 0.016666 penalty 0.069327
## itel    1 lambda   0.110000 stress 0.017295 penalty 0.064380
## itel    1 lambda   0.120000 stress 0.017973 penalty 0.059564
## itel    1 lambda   0.130000 stress 0.018693 penalty 0.054914
## itel    1 lambda   0.140000 stress 0.019446 penalty 0.050458
## itel    1 lambda   0.150000 stress 0.020224 penalty 0.046215
## itel    1 lambda   0.160000 stress 0.021019 penalty 0.042197
## itel    1 lambda   0.170000 stress 0.021824 penalty 0.038412
## itel    1 lambda   0.180000 stress 0.022630 penalty 0.034863
## itel    1 lambda   0.190000 stress 0.023432 penalty 0.031550
## itel    1 lambda   0.200000 stress 0.024224 penalty 0.028472
## itel    1 lambda   0.210000 stress 0.025000 penalty 0.025622
## itel    1 lambda   0.220000 stress 0.025755 penalty 0.022994
## itel    1 lambda   0.230000 stress 0.026487 penalty 0.020581
## itel    1 lambda   0.240000 stress 0.027191 penalty 0.018373
## itel    1 lambda   0.250000 stress 0.027865 penalty 0.016360
## itel    1 lambda   0.260000 stress 0.028506 penalty 0.014530
## itel    1 lambda   0.270000 stress 0.029114 penalty 0.012872
## itel    1 lambda   0.280000 stress 0.029687 penalty 0.011375
## itel    1 lambda   0.290000 stress 0.030225 penalty 0.010027
## itel    1 lambda   0.300000 stress 0.030728 penalty 0.008815
## itel    1 lambda   0.310000 stress 0.031196 penalty 0.007730
## itel    1 lambda   0.320000 stress 0.031630 penalty 0.006761
## itel    1 lambda   0.330000 stress 0.032030 penalty 0.005896
## itel    1 lambda   0.340000 stress 0.032399 penalty 0.005127
## itel    1 lambda   0.350000 stress 0.032736 penalty 0.004445
## itel    1 lambda   0.360000 stress 0.033044 penalty 0.003840
## itel    1 lambda   0.370000 stress 0.033324 penalty 0.003307
## itel    1 lambda   0.380000 stress 0.033578 penalty 0.002836
## itel    1 lambda   0.390000 stress 0.033806 penalty 0.002423
## itel    1 lambda   0.400000 stress 0.034011 penalty 0.002060
## itel    1 lambda   0.410000 stress 0.034195 penalty 0.001744
## itel    1 lambda   0.420000 stress 0.034358 penalty 0.001469
## itel    1 lambda   0.430000 stress 0.034502 penalty 0.001230
## itel    1 lambda   0.440000 stress 0.034629 penalty 0.001024
## itel    1 lambda   0.450000 stress 0.034739 penalty 0.000847
```

```
## itel    1 lambda   0.460000 stress 0.034835 penalty 0.000696
## itel    1 lambda   0.470000 stress 0.034918 penalty 0.000567
## itel    1 lambda   0.480000 stress 0.034989 penalty 0.000459
## itel    1 lambda   0.490000 stress 0.035049 penalty 0.000369
## itel    1 lambda   0.500000 stress 0.035099 penalty 0.000293
## itel    1 lambda   0.510000 stress 0.035141 penalty 0.000231
## itel    1 lambda   0.520000 stress 0.035175 penalty 0.000181
## itel    1 lambda   0.530000 stress 0.035204 penalty 0.000140
## itel    1 lambda   0.540000 stress 0.035226 penalty 0.000107
## itel    1 lambda   0.550000 stress 0.035244 penalty 0.000081
## itel    1 lambda   0.560000 stress 0.035258 penalty 0.000061
## itel    1 lambda   0.570000 stress 0.035269 penalty 0.000045
## itel    1 lambda   0.580000 stress 0.035278 penalty 0.000033
## itel    1 lambda   0.590000 stress 0.035284 penalty 0.000024
## itel    1 lambda   0.600000 stress 0.035289 penalty 0.000017
## itel    1 lambda   0.610000 stress 0.035293 penalty 0.000012
## itel    1 lambda   0.620000 stress 0.035295 penalty 0.000009
## itel    1 lambda   0.630000 stress 0.035297 penalty 0.000006
## itel    1 lambda   0.640000 stress 0.035298 penalty 0.000004
## itel    1 lambda   0.650000 stress 0.035299 penalty 0.000003
## itel    1 lambda   0.660000 stress 0.035300 penalty 0.000002
## itel    1 lambda   0.670000 stress 0.035300 penalty 0.000001
## itel    1 lambda   0.680000 stress 0.035301 penalty 0.000001
## itel    1 lambda   0.690000 stress 0.035301 penalty 0.000001
## itel    1 lambda   0.700000 stress 0.035301 penalty 0.000000
## itel    1 lambda   0.710000 stress 0.035301 penalty 0.000000
## itel    4 lambda   0.720000 stress 0.035301 penalty 0.000000
## itel    3 lambda   0.730000 stress 0.035301 penalty 0.000000
```




```
## itel 1412 lambda   0.000000 stress 0.013675 penalty 0.269308
## itel    5 lambda   0.010000 stress 0.013716 penalty 0.114786
## itel    5 lambda   0.100000 stress 0.016719 penalty 0.069309
## itel   23 lambda   1.000000 stress 0.035301 penalty 0.000000
```

This example was previously analyzed in De Leeuw (2005) using enumeration of all permutations. He found 14354 isolated local minima, and a global minimum equal to the one we computed here.

Plato

Mair, Groenen, and De Leeuw (2022) use seriation of the works of Plato, from the data collected by Cox and Brandwood (1959), as an example of unidimensional scaling.

Using the Torgerson initial configuration in one dimension, smacof finds a stress of 0.1436303539 after 2 iterations.

A full-dimensional scaling with $p = 6$ gives stress $1.525336516 \times 10^{-31}$ after 1 iterations. The singular values of the full dimensional solution are

```
## [1] +0.367934 +0.238357 +0.211808 +0.155444 +0.130119 +0.086998
```

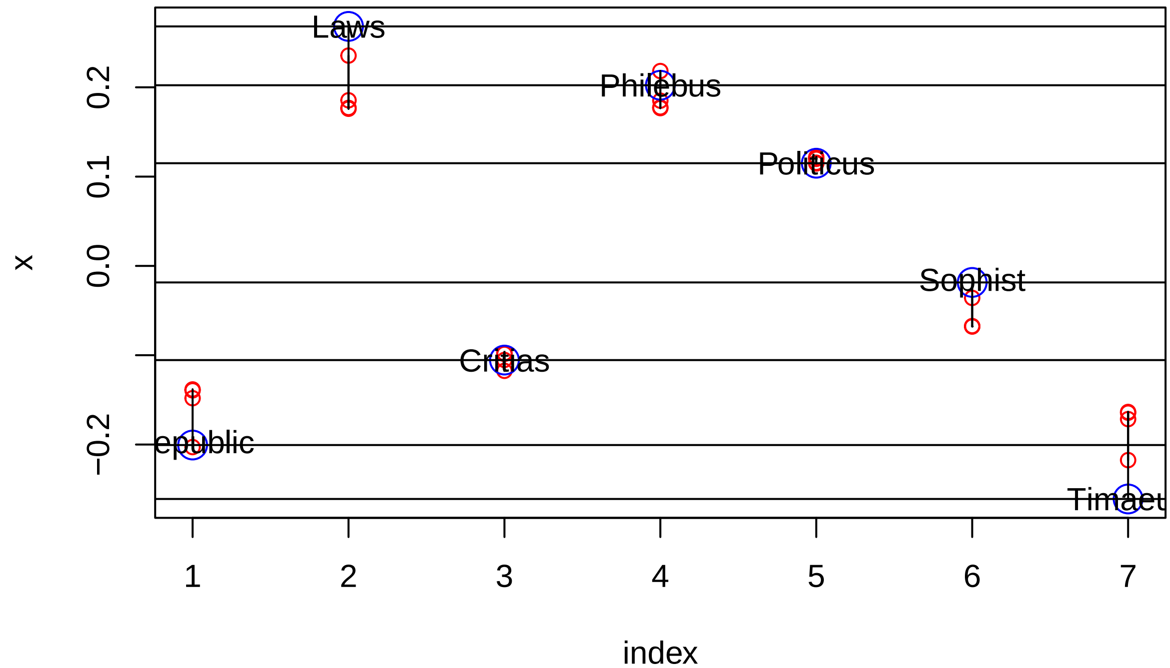
and thus the Gower rank of these (transformed) data is 6.

If we start our smacof iterations with the first dimension of the full dimensional solution stress is 0.1436303539 after 2 iterations, the same solution as with the Torgerson start.

If we run smacof 1000 times with a random start we find 793 local minima. Suffices it to say that the smallest stress is 0.1287689224, which is found in only one of the 1000 runs. It is smaller than stress for the previous Torgerson and FDS solutions.

Now start the global method with a short λ sequence.

```
## itel  169 lambda   0.000000 stress 0.000000 penalty 0.410927
## itel    3 lambda   0.010000 stress 0.000062 penalty 0.255246
## itel    3 lambda   0.100000 stress 0.005117 penalty 0.194993
## itel    4 lambda   1.000000 stress 0.106058 penalty 0.019675
## itel    9 lambda  10.000000 stress 0.139462 penalty 0.000000
```



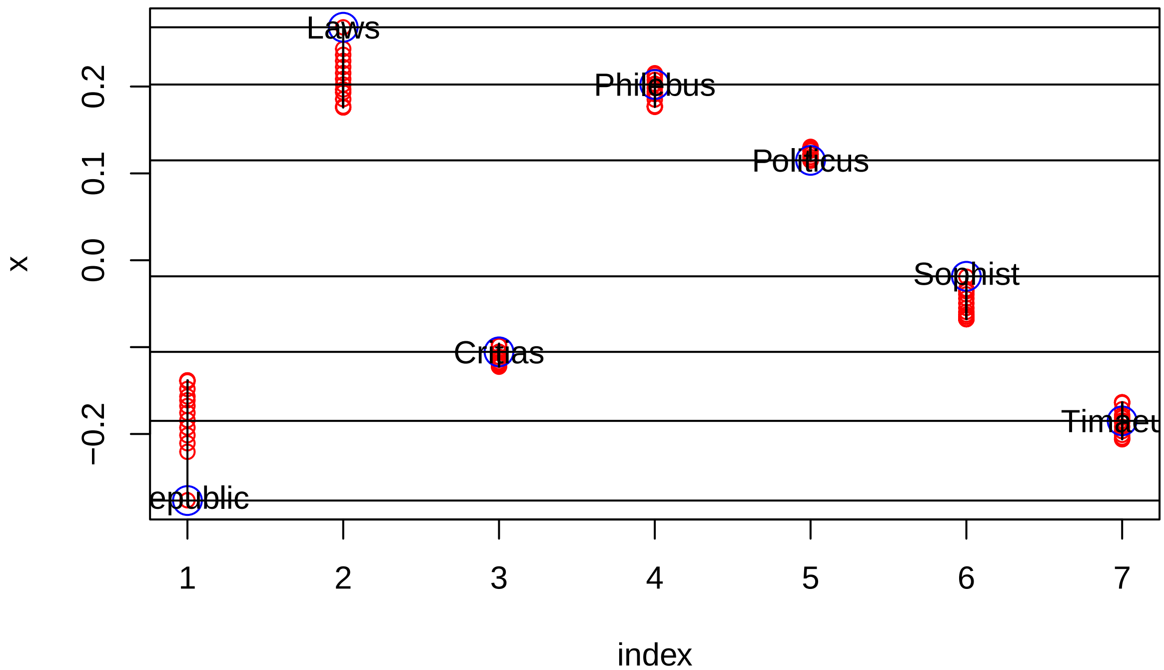
This gives the order

```
##       [,1]
## [1,] "Timaeus"
## [2,] "Republic"
## [3,] "Critias"
## [4,] "Sophist"
## [5,] "Politicus"
## [6,] "Philebus"
## [7,] "Laws"
```

which is different from the order at the global minimum, which has Republic before Timaeus. Thus we have recovered a local minimum, and it seems our sequence of λ values was not fine enough to do the job properly. So we try a longer and finer sequence.

```
## itel  169 lambda   0.000000 stress 0.000000 penalty 0.410927
## itel    3 lambda   0.000100 stress 0.000000 penalty 0.263015
## itel    3 lambda   0.001000 stress 0.000001 penalty 0.262280
## itel    3 lambda   0.010000 stress 0.000064 penalty 0.255078
## itel    3 lambda   0.100000 stress 0.005123 penalty 0.194945
## itel    2 lambda   0.200000 stress 0.016184 penalty 0.147493
```

```
## itel    1 lambda   0.300000 stress 0.026997 penalty 0.119323
## itel    1 lambda   0.400000 stress 0.040023 penalty 0.093615
## itel    1 lambda   0.500000 stress 0.053688 penalty 0.072330
## itel    1 lambda   0.600000 stress 0.066833 penalty 0.055452
## itel    1 lambda   0.700000 stress 0.078832 penalty 0.042269
## itel    1 lambda   0.800000 stress 0.089439 penalty 0.032019
## itel    1 lambda   0.900000 stress 0.098557 penalty 0.024079
## itel    1 lambda   1.000000 stress 0.106135 penalty 0.017940
## itel    6 lambda   2.000000 stress 0.130789 penalty 0.000148
## itel   13 lambda   3.000000 stress 0.131135 penalty 0.000000
```



Now the order is

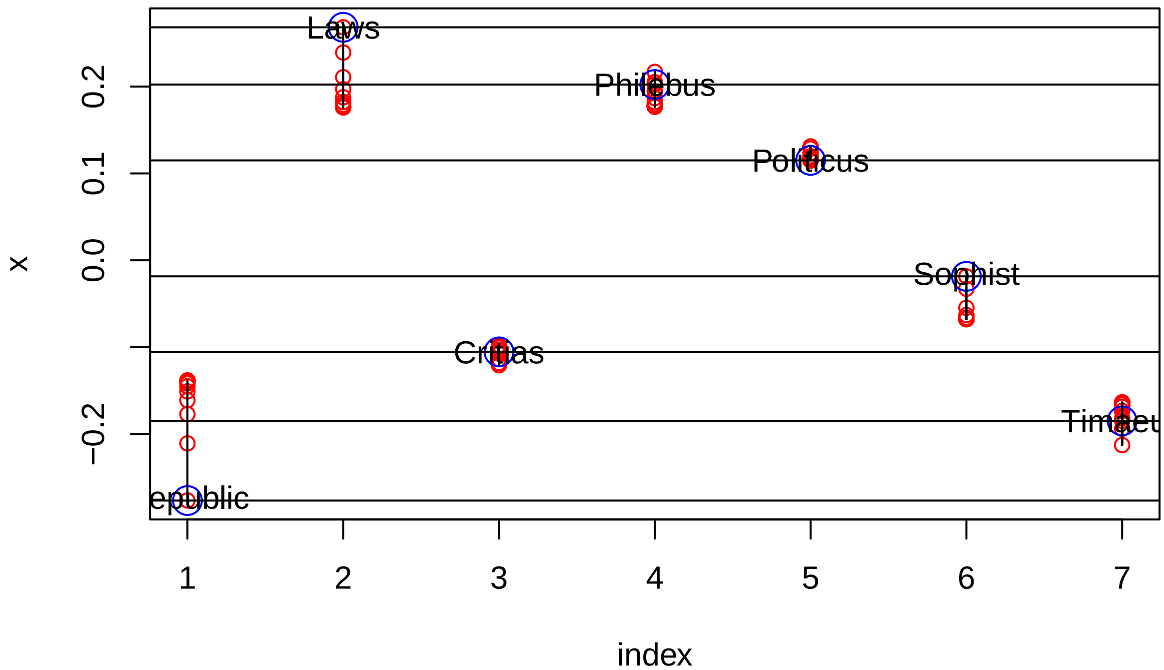
```
##      [,1]
## [1,] "Republic"
## [2,] "Timaeus"
## [3,] "Critias"
## [4,] "Sophist"
## [5,] "Politicus"
## [6,] "Philebus"
## [7,] "Laws"
```

which does indeed correspond to the global minimum.

With a different λ sequence we find the same solution.

```
## itel  169 lambda   0.000000 stress 0.000000 penalty 0.410927
## itel    3 lambda   0.001000 stress 0.000001 penalty 0.262296
## itel    2 lambda   0.002000 stress 0.000003 penalty 0.261483
```

```
## itel    2 lambda   0.004000 stress 0.000010 penalty 0.259872
## itel    2 lambda   0.008000 stress 0.000041 penalty 0.256690
## itel    2 lambda   0.016000 stress 0.000159 penalty 0.250470
## itel    2 lambda   0.032000 stress 0.000613 penalty 0.238574
## itel    2 lambda   0.064000 stress 0.002266 penalty 0.216785
## itel    2 lambda   0.128000 stress 0.007791 penalty 0.180067
## itel    2 lambda   0.256000 stress 0.023483 penalty 0.127006
## itel    2 lambda   0.512000 stress 0.056940 penalty 0.067948
## itel    3 lambda   1.024000 stress 0.107743 penalty 0.017937
## itel    8 lambda   2.048000 stress 0.131059 penalty 0.000032
## itel    9 lambda   4.096000 stress 0.131135 penalty 0.000000
```



The order is

```
##       [,1]
## [1,] "Republic"
## [2,] "Timaeus"
## [3,] "Critias"
## [4,] "Sophist"
## [5,] "Politicus"
## [6,] "Philebus"
## [7,] "Laws"
```

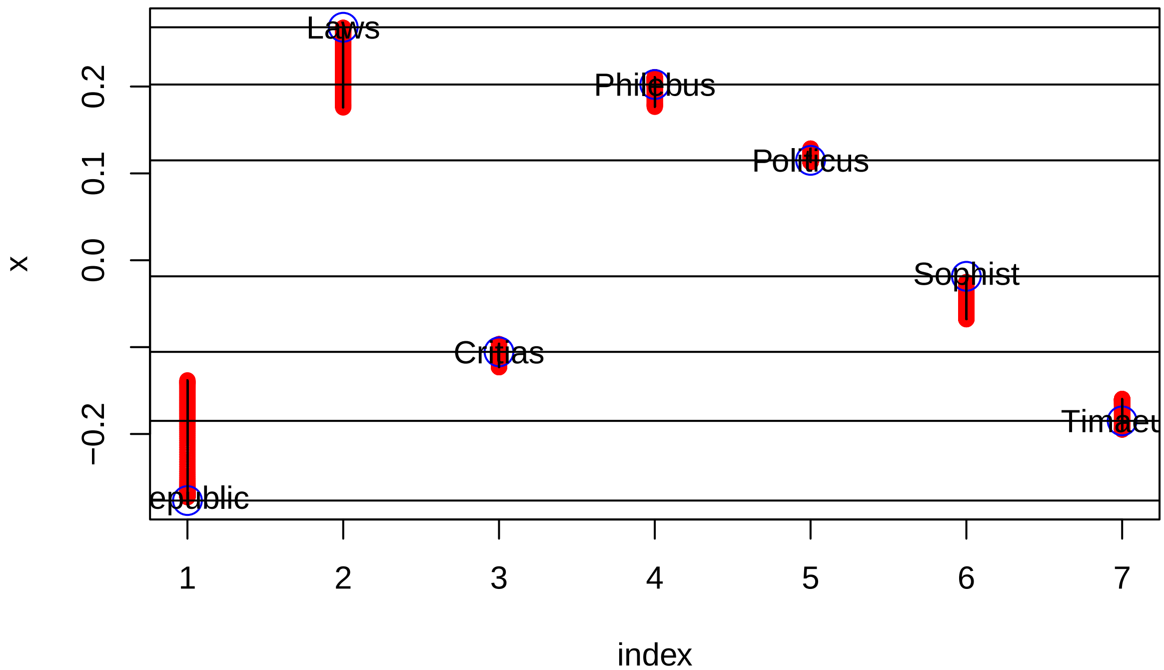
Our global optimization method with the default λ sequence also converges to the same smallest local minimum.

```
## itel  169 lambda   0.000000 stress 0.000000 penalty 0.410927
## itel    3 lambda   0.010000 stress 0.000062 penalty 0.255246
## itel    2 lambda   0.020000 stress 0.000245 penalty 0.247505
```

```
## itel    1 lambda   0.030000 stress 0.000488 penalty 0.241370
## itel    1 lambda   0.040000 stress 0.000859 penalty 0.234376
## itel    1 lambda   0.050000 stress 0.001366 penalty 0.226943
## itel    1 lambda   0.060000 stress 0.002009 penalty 0.219341
## itel    1 lambda   0.070000 stress 0.002784 penalty 0.211742
## itel    1 lambda   0.080000 stress 0.003684 penalty 0.204257
## itel    1 lambda   0.090000 stress 0.004698 penalty 0.196954
## itel    1 lambda   0.100000 stress 0.005816 penalty 0.189875
## itel    1 lambda   0.110000 stress 0.007025 penalty 0.183041
## itel    1 lambda   0.120000 stress 0.008317 penalty 0.176460
## itel    1 lambda   0.130000 stress 0.009682 penalty 0.170134
## itel    1 lambda   0.140000 stress 0.011110 penalty 0.164057
## itel    1 lambda   0.150000 stress 0.012594 penalty 0.158222
## itel    1 lambda   0.160000 stress 0.014128 penalty 0.152618
## itel    1 lambda   0.170000 stress 0.015704 penalty 0.147236
## itel    1 lambda   0.180000 stress 0.017317 penalty 0.142064
## itel    1 lambda   0.190000 stress 0.018962 penalty 0.137093
## itel    1 lambda   0.200000 stress 0.020635 penalty 0.132311
## itel    1 lambda   0.210000 stress 0.022331 penalty 0.127710
## itel    1 lambda   0.220000 stress 0.024047 penalty 0.123281
## itel    1 lambda   0.230000 stress 0.025780 penalty 0.119015
## itel    1 lambda   0.240000 stress 0.027525 penalty 0.114904
## itel    1 lambda   0.250000 stress 0.029281 penalty 0.110941
## itel    1 lambda   0.260000 stress 0.031045 penalty 0.107118
## itel    1 lambda   0.270000 stress 0.032814 penalty 0.103430
## itel    1 lambda   0.280000 stress 0.034587 penalty 0.099869
## itel    1 lambda   0.290000 stress 0.036361 penalty 0.096430
## itel    1 lambda   0.300000 stress 0.038136 penalty 0.093107
## itel    1 lambda   0.310000 stress 0.039909 penalty 0.089895
## itel    1 lambda   0.320000 stress 0.041680 penalty 0.086788
## itel    1 lambda   0.330000 stress 0.043447 penalty 0.083781
## itel    1 lambda   0.340000 stress 0.045209 penalty 0.080870
## itel    1 lambda   0.350000 stress 0.046965 penalty 0.078050
## itel    1 lambda   0.360000 stress 0.048715 penalty 0.075317
## itel    1 lambda   0.370000 stress 0.050458 penalty 0.072666
## itel    1 lambda   0.380000 stress 0.052193 penalty 0.070095
## itel    1 lambda   0.390000 stress 0.053920 penalty 0.067598
## itel    1 lambda   0.400000 stress 0.055637 penalty 0.065173
## itel    1 lambda   0.410000 stress 0.057344 penalty 0.062816
## itel    1 lambda   0.420000 stress 0.059042 penalty 0.060524
## itel    1 lambda   0.430000 stress 0.060728 penalty 0.058295
## itel    1 lambda   0.440000 stress 0.062404 penalty 0.056125
## itel    1 lambda   0.450000 stress 0.064068 penalty 0.054012
## itel    1 lambda   0.460000 stress 0.065721 penalty 0.051953
## itel    1 lambda   0.470000 stress 0.067362 penalty 0.049946
```

```
## itel    1 lambda   0.480000 stress 0.068991 penalty 0.047990
## itel    1 lambda   0.490000 stress 0.070607 penalty 0.046082
## itel    1 lambda   0.500000 stress 0.072211 penalty 0.044222
## itel    1 lambda   0.510000 stress 0.073802 penalty 0.042410
## itel    1 lambda   0.520000 stress 0.075378 penalty 0.040646
## itel    1 lambda   0.530000 stress 0.076938 penalty 0.038931
## itel    1 lambda   0.540000 stress 0.078479 penalty 0.037266
## itel    1 lambda   0.550000 stress 0.079999 penalty 0.035654
## itel    1 lambda   0.560000 stress 0.081496 penalty 0.034096
## itel    1 lambda   0.570000 stress 0.082965 penalty 0.032594
## itel    1 lambda   0.580000 stress 0.084405 penalty 0.031150
## itel    1 lambda   0.590000 stress 0.085811 penalty 0.029765
## itel    1 lambda   0.600000 stress 0.087182 penalty 0.028440
## itel    1 lambda   0.610000 stress 0.088516 penalty 0.027174
## itel    1 lambda   0.620000 stress 0.089811 penalty 0.025966
## itel    1 lambda   0.630000 stress 0.091066 penalty 0.024817
## itel    1 lambda   0.640000 stress 0.092280 penalty 0.023725
## itel    1 lambda   0.650000 stress 0.093453 penalty 0.022689
## itel    1 lambda   0.660000 stress 0.094584 penalty 0.021706
## itel    1 lambda   0.670000 stress 0.095675 penalty 0.020775
## itel    1 lambda   0.680000 stress 0.096726 penalty 0.019895
## itel    1 lambda   0.690000 stress 0.097737 penalty 0.019062
## itel    1 lambda   0.700000 stress 0.098709 penalty 0.018275
## itel    1 lambda   0.710000 stress 0.099645 penalty 0.017532
## itel    1 lambda   0.720000 stress 0.100545 penalty 0.016830
## itel    1 lambda   0.730000 stress 0.101411 penalty 0.016166
## itel    1 lambda   0.740000 stress 0.102244 penalty 0.015540
## itel    1 lambda   0.750000 stress 0.103046 penalty 0.014947
## itel    1 lambda   0.760000 stress 0.103818 penalty 0.014387
## itel    1 lambda   0.770000 stress 0.104563 penalty 0.013856
## itel    1 lambda   0.780000 stress 0.105280 penalty 0.013354
## itel    1 lambda   0.790000 stress 0.105972 penalty 0.012877
## itel    1 lambda   0.800000 stress 0.106641 penalty 0.012425
## itel    1 lambda   0.810000 stress 0.107286 penalty 0.011995
## itel    1 lambda   0.820000 stress 0.107909 penalty 0.011587
## itel    1 lambda   0.830000 stress 0.108510 penalty 0.011198
## itel    1 lambda   0.840000 stress 0.109092 penalty 0.010828
## itel    1 lambda   0.850000 stress 0.109655 penalty 0.010476
## itel    1 lambda   0.860000 stress 0.110199 penalty 0.010140
## itel    1 lambda   0.870000 stress 0.110726 penalty 0.009819
## itel    1 lambda   0.880000 stress 0.111236 penalty 0.009513
## itel    1 lambda   0.890000 stress 0.111731 penalty 0.009220
## itel    1 lambda   0.900000 stress 0.112210 penalty 0.008940
## itel    1 lambda   0.910000 stress 0.112676 penalty 0.008672
## itel    1 lambda   0.920000 stress 0.113129 penalty 0.008414
```

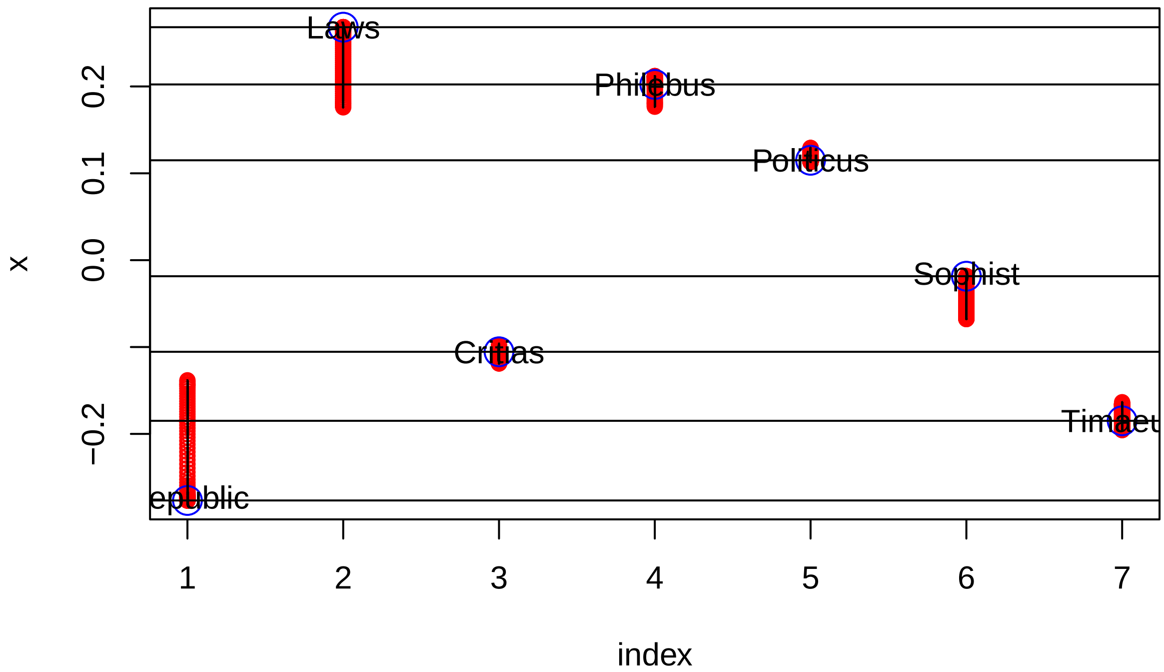
```
## itel    1 lambda   0.930000 stress 0.113570 penalty 0.008166
## itel    1 lambda   0.940000 stress 0.114001 penalty 0.007928
## itel    1 lambda   0.950000 stress 0.114422 penalty 0.007697
## itel    1 lambda   0.960000 stress 0.114834 penalty 0.007474
## itel    1 lambda   0.970000 stress 0.115238 penalty 0.007258
## itel    1 lambda   0.980000 stress 0.115637 penalty 0.007047
## itel    1 lambda   0.990000 stress 0.116030 penalty 0.006841
## itel    1 lambda   1.000000 stress 0.116419 penalty 0.006639
## itel    1 lambda   2.000000 stress 0.124820 penalty 0.002891
## itel   11 lambda   5.000000 stress 0.131135 penalty 0.000000
```




```
## itel  169 lambda   0.000000 stress 0.000000 penalty 0.410927
## itel    3 lambda   0.020000 stress 0.000241 penalty 0.247687
## itel    2 lambda   0.040000 stress 0.000932 penalty 0.233031
## itel    1 lambda   0.060000 stress 0.001815 penalty 0.221839
## itel    1 lambda   0.080000 stress 0.003123 penalty 0.209450
## itel    1 lambda   0.100000 stress 0.004849 penalty 0.196723
## itel    1 lambda   0.120000 stress 0.006964 penalty 0.184174
## itel    1 lambda   0.140000 stress 0.009420 penalty 0.172104
## itel    1 lambda   0.160000 stress 0.012159 penalty 0.160674
## itel    1 lambda   0.180000 stress 0.015125 penalty 0.149951
## itel    1 lambda   0.200000 stress 0.018264 penalty 0.139947
## itel    1 lambda   0.220000 stress 0.021533 penalty 0.130640
## itel    1 lambda   0.240000 stress 0.024892 penalty 0.121988
## itel    1 lambda   0.260000 stress 0.028312 penalty 0.113946
## itel    1 lambda   0.280000 stress 0.031767 penalty 0.106464
## itel    1 lambda   0.300000 stress 0.035236 penalty 0.099496
```

```
## itel    1 lambda   0.320000 stress 0.038704 penalty 0.092999
## itel    1 lambda   0.340000 stress 0.042155 penalty 0.086932
## itel    1 lambda   0.360000 stress 0.045579 penalty 0.081260
## itel    1 lambda   0.380000 stress 0.048967 penalty 0.075949
## itel    1 lambda   0.400000 stress 0.052311 penalty 0.070970
## itel    1 lambda   0.420000 stress 0.055605 penalty 0.066295
## itel    1 lambda   0.440000 stress 0.058844 penalty 0.061900
## itel    1 lambda   0.460000 stress 0.062024 penalty 0.057764
## itel    1 lambda   0.480000 stress 0.065139 penalty 0.053866
## itel    1 lambda   0.500000 stress 0.068188 penalty 0.050188
## itel    1 lambda   0.520000 stress 0.071166 penalty 0.046713
## itel    1 lambda   0.540000 stress 0.074073 penalty 0.043424
## itel    1 lambda   0.560000 stress 0.076907 penalty 0.040305
## itel    1 lambda   0.580000 stress 0.079668 penalty 0.037343
## itel    1 lambda   0.600000 stress 0.082358 penalty 0.034526
## itel    1 lambda   0.620000 stress 0.084977 penalty 0.031847
## itel    1 lambda   0.640000 stress 0.087524 penalty 0.029303
## itel    1 lambda   0.660000 stress 0.089994 penalty 0.026899
## itel    1 lambda   0.680000 stress 0.092378 penalty 0.024644
## itel    1 lambda   0.700000 stress 0.094662 penalty 0.022549
## itel    1 lambda   0.720000 stress 0.096833 penalty 0.020623
## itel    1 lambda   0.740000 stress 0.098879 penalty 0.018867
## itel    1 lambda   0.760000 stress 0.100796 penalty 0.017278
## itel    1 lambda   0.780000 stress 0.102584 penalty 0.015847
## itel    1 lambda   0.800000 stress 0.104247 penalty 0.014562
## itel    1 lambda   0.820000 stress 0.105793 penalty 0.013409
## itel    1 lambda   0.840000 stress 0.107231 penalty 0.012374
## itel    1 lambda   0.860000 stress 0.108569 penalty 0.011444
## itel    1 lambda   0.880000 stress 0.109818 penalty 0.010607
## itel    1 lambda   0.900000 stress 0.110985 penalty 0.009852
## itel    1 lambda   0.920000 stress 0.112078 penalty 0.009168
## itel    1 lambda   0.940000 stress 0.113105 penalty 0.008546
## itel    1 lambda   0.960000 stress 0.114072 penalty 0.007979
## itel    1 lambda   0.980000 stress 0.114987 penalty 0.007459
## itel    1 lambda   1.000000 stress 0.115855 penalty 0.006980
## itel    1 lambda   1.020000 stress 0.116682 penalty 0.006536
## itel    1 lambda   1.040000 stress 0.117474 penalty 0.006122
## itel    1 lambda   1.060000 stress 0.118237 penalty 0.005732
## itel    1 lambda   1.080000 stress 0.118975 penalty 0.005363
## itel    1 lambda   1.100000 stress 0.119693 penalty 0.005010
## itel    1 lambda   1.120000 stress 0.120395 penalty 0.004671
## itel    1 lambda   1.140000 stress 0.121086 penalty 0.004343
## itel    1 lambda   1.160000 stress 0.121766 penalty 0.004024
## itel    1 lambda   1.180000 stress 0.122438 penalty 0.003713
## itel    1 lambda   1.200000 stress 0.123101 penalty 0.003410
```

```
## itel    1 lambda   1.220000 stress 0.123755 penalty 0.003114
## itel    1 lambda   1.240000 stress 0.124397 penalty 0.002826
## itel    1 lambda   1.260000 stress 0.125024 penalty 0.002549
## itel    1 lambda   1.280000 stress 0.125632 penalty 0.002283
## itel    1 lambda   1.300000 stress 0.126217 penalty 0.002029
## itel    1 lambda   1.320000 stress 0.126775 penalty 0.001790
## itel    1 lambda   1.340000 stress 0.127301 penalty 0.001567
## itel    1 lambda   1.360000 stress 0.127793 penalty 0.001360
## itel    1 lambda   1.380000 stress 0.128249 penalty 0.001170
## itel    1 lambda   1.400000 stress 0.128667 penalty 0.000997
## itel    1 lambda   1.420000 stress 0.129046 penalty 0.000841
## itel    1 lambda   1.440000 stress 0.129386 penalty 0.000702
## itel    1 lambda   1.460000 stress 0.129687 penalty 0.000580
## itel    1 lambda   1.480000 stress 0.129950 penalty 0.000473
## itel    1 lambda   1.500000 stress 0.130177 penalty 0.000382
## itel    1 lambda   1.520000 stress 0.130371 penalty 0.000304
## itel    1 lambda   1.540000 stress 0.130533 penalty 0.000239
## itel    1 lambda   1.560000 stress 0.130667 penalty 0.000186
## itel    1 lambda   1.580000 stress 0.130776 penalty 0.000142
## itel    1 lambda   1.600000 stress 0.130864 penalty 0.000107
## itel    1 lambda   1.620000 stress 0.130933 penalty 0.000080
## itel    1 lambda   1.640000 stress 0.130987 penalty 0.000059
## itel    1 lambda   1.660000 stress 0.131028 penalty 0.000042
## itel    1 lambda   1.680000 stress 0.131058 penalty 0.000030
## itel    1 lambda   1.700000 stress 0.131081 penalty 0.000021
## itel    1 lambda   1.720000 stress 0.131098 penalty 0.000015
## itel    1 lambda   1.740000 stress 0.131109 penalty 0.000010
## itel    1 lambda   1.760000 stress 0.131118 penalty 0.000007
## itel    1 lambda   1.780000 stress 0.131123 penalty 0.000004
## itel    1 lambda   1.800000 stress 0.131127 penalty 0.000003
## itel    1 lambda   1.820000 stress 0.131130 penalty 0.000002
## itel    1 lambda   1.840000 stress 0.131132 penalty 0.000001
## itel    1 lambda   1.860000 stress 0.131133 penalty 0.000001
## itel    1 lambda   1.880000 stress 0.131134 penalty 0.000000
## itel    1 lambda   1.900000 stress 0.131134 penalty 0.000000
## itel    1 lambda   1.920000 stress 0.131134 penalty 0.000000
## itel    1 lambda   1.940000 stress 0.131134 penalty 0.000000
## itel    1 lambda   1.960000 stress 0.131135 penalty 0.000000
## itel    1 lambda   1.980000 stress 0.131135 penalty 0.000000
## itel    1 lambda   2.000000 stress 0.131135 penalty 0.000000
## itel    1 lambda   2.020000 stress 0.131135 penalty 0.000000
## itel    1 lambda   2.040000 stress 0.131135 penalty 0.000000
```

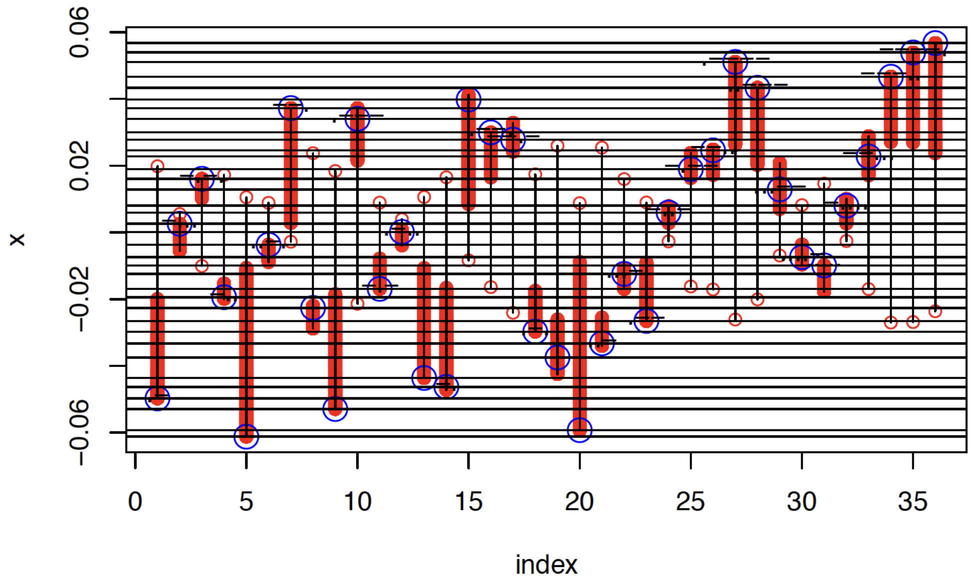


Morse in One

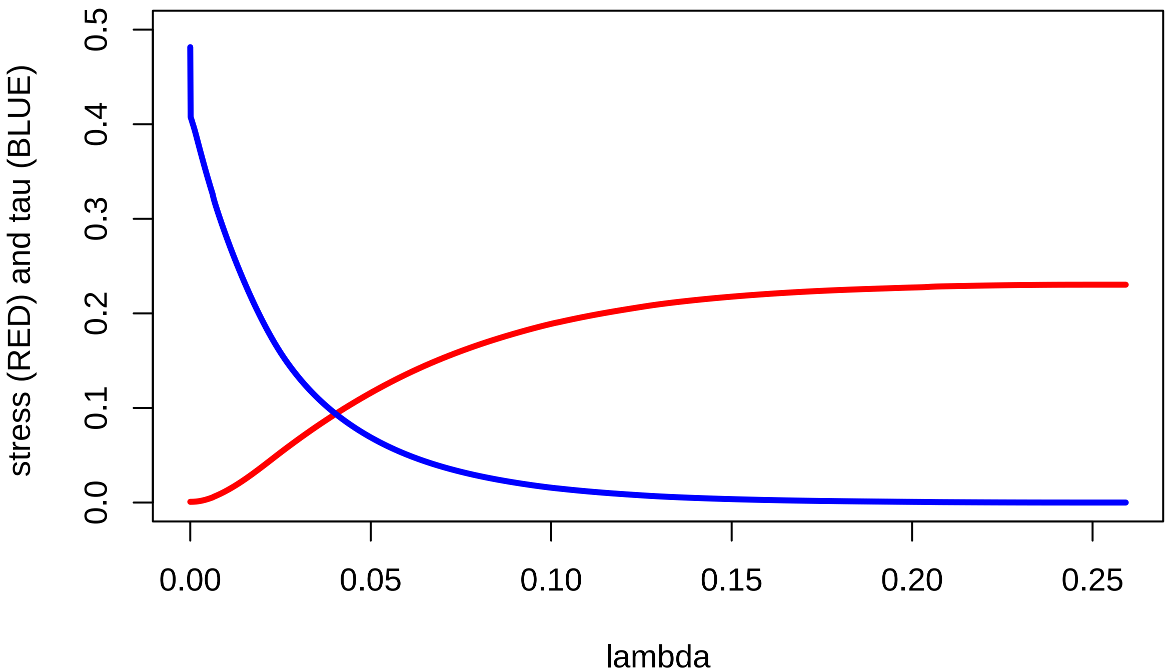
Now for a more challenging example. The Morse code data have been used to try out exact unidimensional MDS techniques, for example by Palubeckis (2013). We will enter the global minimum contest by using 10,000 values of λ, in an equally spaced sequence from 0 to 10. This is not as bad as it sounds. For the 10,000 FDS solutions `system.time()` tells us

```
##    user  system elapsed
##  26.729   1.063  28.107
```

The one-dimensional plot show quite a bit of movement, but much of it seems to be contained in the very first change of λ.



We can also plot stress and the penalty term as functions of λ. Again, note the big change in the penalty term when λ goes from zero to 0.001.



After the first 2593 values of λ the penalty term is zero and we stop, i.e. we estimate λ_+ is 2.593. At that point we have run a total of 5013 FDS iterations, and thus on average about two iterations per λ value. Stress has increased from 0.0007634501 to 0.2303106976 and the penalty value has decreased from 0.4815136419 to 0.0000000001. We find the following order of the points on the dimension.

```
##       [,1]
##  [1,] "."
```

```
##  [2,] "-"
##  [3,] ".."
##  [4,] ".-"
##  [5,] "-."
##  [6,] "--"
##  [7,] "..."
##  [8,] "..-"
##  [9,] ".-."
## [10,] ".--"
## [11,] "...."
## [12,] "-.."
## [13,] "-.-"
## [14,] "...-"
## [15,] "....."
## [16,] "....-"
## [17,] "..-."
## [18,] ".-.."
## [19,] "-..."
## [20,] "-..-"
## [21,] "-...."
## [22,] "...--"
## [23,] "-.-."
## [24,] "-.--"
## [25,] "--..."
## [26,] "--.."
## [27,] "--.-"
## [28,] ".--."
## [29,] ".---"
## [30,] "--."
## [31,] "---"
## [32,] "..---"
## [33,] "---.."
## [34,] ".----"
## [35,] "----."
## [36,] "-----"
```

Our order, and consequently our solution, is the same as the exact global solution given by Palubeckis (2013). See his table 4, reproduced below. The difference is that computing our solution takes 10 seconds, while his takes 494 seconds. But of course we would not know we actually found the global mimimum if the exact exhaustive methods had not analyzed the same data before.

TABLE 4: Optimal solutions for the full Morse code dissimilarity matrix and th

i	Morse code full	
	$p(i)$	$x_{p(i)}$
1	(E) •	0.00000
2	(T) –	5.83333
3	(I) ••	24.77778
4	(A) •–	34.08333
5	(N) –•	44.11111
6	(M) – –	52.33333
7	(S) • • •	70.30556
8	(U) • • –	83.13889
9	(R) • – •	93.47222
10	(W) • – –	102.97222
11	(H) • • ••	114.44444
12	(D) – • •	124.30556
13	(K) – • –	131.52778
14	(V) • • •–	145.00000
15	(5) • • • • •	152.44444
16	(4) • • • • –	159.91667
17	(F) • • –•	170.75000
18	(L) • – ••	182.25000
19	(B) – • ••	189.52778
20	(X) – • •–	199.55556
21	(6) – • • • •	205.66667
22	(3) • • • – –	220.13889
23	(C) – • –•	229.47222
24	(Y) – • ––	238.41667
25	(7) – – • • •	249.30556
26	(Z) – – ••	254.88889
27	(Q) – – •–	264.38889
28	(P) • – –•	270.83333
29	(J) • – ––	282.94444
30	(G) – – •	292.47222
31	(O) – – –	300.22222
32	(2) • • – – –	310.50000
33	(8) – – – • •	320.36111
34	(1) • – – – –	333.50000
35	(9) – – – – •	341.86111
36	(0) – – – – –	350.27778

Discussion

There is one surprising (to me, at least) finding from all our examples. There is a value, say λ_+, such that the penalty $\tau(Y)$ is zero for all PFDS solutions with $\lambda \geq \lambda_+$. In other words, our penalty function acts like a *smooth exact penalty function.* The precise reason for exactness in our case (if there is one) is not entirely clear to me yet, but it is obviously a topic for further research, using for example the recent theoretical framework of Dolgopolik (2016a), Dolgopolik (2016b), Dolgopolik (2017), Dolgopolik (n.d.).

In our two dimensional examples we always start our plots with the first two dimensions of the FDS configuration. These two-dimensional configurations are usually small (all points relatively close to the origin), because so much variation is still in the higher dimensions. If λ increases the growth of the configurations is one important aspect of configuration change.

In our iteration counts with short sequences of λ we see relatively small increases in stress and small decreases in the penalty term, until we get closer to λ_+, when we suddenly see a sudden change and a larger number of iterations. This is also reflected in the figures, where generally the change to the last solution (with the largest λ) makes the largest jump. This suggest a finer sequence near λ_+ and perhaps an adaptive strategy for choosing λ. Or to use brute force, as in the unidimensional Morse code example. With such longer and finer sequences convergence becomes more smooth.

Another all-important aspect of the method discussed here is that it assumes computation of the global minimum for each λ. Since we cannot expect a result as nice as the one for FDS (all local minima are global) for $\lambda > 0$ our method remains somewhat heuristic. We have seen that some sequences of λ can take us to a non-global local minimum. Of course the fact that we start with a global minimum for $\lambda = 0$ is of some help, but we do not know how far it will take us in general. Jumps near λ_+ may indicate bifurcations to other local minima.

We have not stressed in the paper that minimizing the penalty function is a *continuation method* (Allgower and George (1979)). This means that probably better methods are available to follow the trajectory of solutions along $\lambda > 0$. There are also possibilities in exploring the fact that the maximum over Z of the penalty function (12) is a concave function of the single variable λ, which is a constant function for all $\lambda > \lambda_+$. There is a duality theory associated with these Courant penalty functions, which we have not used or explored so far.

Appendix A: Exterior Penalty Methods

Suppose $\mathcal{X} \subseteq \mathbb{R}^n$ and $f : \mathbb{R}^n \Rightarrow \mathbb{R}$ is continuous. Define

$$\mathcal{X}_\star = \underset{x \in \mathcal{X}}{\operatorname{argmin}}\ f(x)$$

Suppose $\mathcal{X}_\star$ is non-empty and that $x_\star$ is any element of $\mathcal{X}_\star$, and

$$f_\star = f(x_\star) = \min_{x \in \mathcal{X}}\ f(x).$$

The following convergence analysis of external linear penalty methods is standard and can be found in many texts (for example, Zangwill (1969), section 12.2).

The penalty term $g : \mathbb{R}^n \Rightarrow \mathbb{R}^+$ is continuous and satisfies $g(x) = 0$ if and only if $x \in \mathcal{X}$. For each $\lambda > 0$ we define the (linear, external) penalty function

$$h(x, \lambda) = f(x) + \lambda g(x). \tag{18}$$

Suppose $\{\lambda_k\}$ is a strictly increasing sequence of positive real numbers. Define

$$\mathcal{X}_k = \underset{x \in \mathcal{X}}{\operatorname{argmin}}\ h(x, \lambda_k). \tag{19}$$

Suppose all $\mathcal{X}_k$ are nonempty and contained in a compact subset of $\mathcal{X}$. Choose $x_k \in \mathcal{X}_k$ arbitrarily.

Lemma 2: [Basic]

1: $h(x_k, \lambda_k) \leq h(x_{k+1}, \lambda_{k+1})$.

2: $g(x_k) \geq g(x_{k+1})$.

3: $f(x_k) \leq f(x_{k+1})$.

4: $f_\star \geq h(x_k, \lambda_k) \geq f(x_k)$.

Proof:

1: We have the chain

$$h(x_{k+1}, \lambda_{k+1}) = f(x_{k+1}) + \lambda_{k+1} g(x_{k+1}) \geq f(x_{k+1}) + \lambda_k g(x_{k+1}) \geq f(x_k) + \lambda_k g(x_k) = h(x_k, \lambda_k).$$

2: Both

$$f(x_k) + \lambda_k g(x_k) \leq f(x_{k+1}) + \lambda_k g(x_{k+1}), \tag{20}$$
$$f(x_{k+1}) + \lambda_{k+1} g(x_{k+1}) \leq f(x_k) + \lambda_{k+1} g(x_k). \tag{21}$$

Adding inequalities (20) and (21) gives

$$\lambda_k g(x_k) + \lambda_{k+1} g(x_{k+1}) \leq \lambda_k g(x_{k+1}) + \lambda_{k+1} g(x_k),$$

or

$$(\lambda_k - \lambda_{k+1}) g(x_k) \leq (\lambda_k - \lambda_{k+1}) g(x_{k+1}),$$

and thus $g(x_k) \geq g(x_{k+1})$.

3: First

$$f(x_{k+1}) + \lambda_k g(x_{k+1}) \geq f(x_k) + \lambda_k g(x_k). \tag{22}$$

We just proved that $g(x_{k+1}) \geq g(x_k)$, and thus

$$f(x_k) + \lambda_k g(x_k) \geq f(x_k) + \lambda_k g(x_{k+1}). \tag{23}$$

Combining inequalities (22) and (23) gives $f(x_{k+1}) \geq f(x_k)$.

4: We have the chain

$$f_\star = f(x_\star) + \lambda_k g(x_\star) \geq f(x_k) + \lambda_k g(x_k) \geq f(x_k).$$

■

Theorem 3: Suppose the sequence $\{\lambda_k\}_{k \in K}$ diverges to ∞ and $x_{\star\star}$ is the limit of any convergent subsequence $\{x_\ell\}_{\ell \in L}$. Then $x_{\star\star} \in \mathcal{X}_\star$, and $f(x_{\star\star}) = f_\star$, and $g(x_{\star\star}) = 0$.

Proof: Using part 4 of lemma 2

$$\lim_{\ell \in L} h(x_\ell, \lambda_\ell) = \lim_{\ell \in L} \{f(x_\ell) + \lambda_\ell g(x_\ell)\} = f(x_{\star\star}) + \lim_{\ell \in L} \lambda_\ell g(x_\ell) \leq f(x_\star).$$

Thus $\{h(x_\ell, \lambda_\ell)_{\ell \in L}\}$ is a bounded increasing sequence, which consequently converges, and $\lim_{\ell \in L} \lambda_\ell g(x_\ell)$ also converges. Since $\{\lambda_\ell\}_{\ell \in L} \rightarrow \infty$ it follows that $\lim_{\ell \in L} g(x_\ell) = g(x_{\star\star}) = 0$. Thus $x_{\star\star} \in \mathcal{X}$. Since $f(x_\ell) \leq f_\star$ we see that $f(x_{\star\star}) \leq f_\star$, and thus $x_{\star\star} \in \mathcal{X}_\star$ and $f(x_{\star\star}) = f_\star$. ■

Appendix B: Code

penalty.R

```
source("smacofBasics.R")

smacofComplement <- function(y, v) {
  return(sum(v * tcrossprod(y)) / 4)
}

smacofPenalty <-
  function(w,
           delta,
           p = 2,
           lbd = 0,
           zold = columnCenter(diag(nrow(delta))),
           itmax = 10000,
           eps = 1e-10,
           verbose = FALSE) {
    itel <- 1
    n <- nrow(zold)
    vmat <- smacofVmat(w)
    vinv <- solve(vmat + (1 / n)) - (1 / n)
    dold <- as.matrix(dist(zold))
    mold <- sum(w * delta * dold) / sum(w * dold * dold)
    zold <- zold * mold
    dold <- dold * mold
    yold <- zold[, (p + 1):n]
    sold <- smacofLoss(dold, w, delta)
    bold <- smacofBmat(dold, w, delta)
    told <- smacofComplement(yold, vmat)
    uold <- sold + lbd * told
    repeat {
      znew <- smacofGuttman(zold, bold, vinv)
      ynew <- znew[, (p + 1):n] / (1 + lbd)
```

```r
    znew[, (p + 1):n] <- ynew
    xnew <- znew[, 1:p]
    dnew <- as.matrix(dist(znew))
    bnew <- smacofBmat(dnew, w, delta)
    tnew <- smacofComplement(ynew, vmat)
    snew <- smacofLoss(dnew, w, delta)
    unew <- snew + lbd * tnew
    if (verbose) {
      cat(
        "itel ",
        formatC(itel, width = 4, format = "d"),
        "sold ",
        formatC(
          sold,
          width = 10,
          digits = 6,
          format = "f"
        ),
        "snew ",
        formatC(
          snew,
          width = 10,
          digits = 6,
          format = "f"
        ),
        "told ",
        formatC(
          told,
          width = 10,
          digits = 6,
          format = "f"
        ),
        "tnew ",
        formatC(
          tnew,
          width = 10,
          digits = 6,
          format = "f"
        ),
        "uold ",
        formatC(
          uold,
          width = 10,
          digits = 6,
```

```
          format = "f"
        ),
        "unew ",
        formatC(
          unew,
          width = 10,
          digits = 6,
          format = "f"
        ),
        "\n"
      )
    }
    if (((uold - unew) < eps) || (itel == itmax)) {
      break
    }
    itel <- itel + 1
    zold <- znew
    bold <- bnew
    sold <- snew
    told <- tnew
    uold <- unew
  }
  zpri <- znew %*% svd(znew)$v
  xpri <- zpri[, 1:p]
  return(list(
    x = xpri,
    z = zpri,
    b = bnew,
    l = lbd,
    s = snew,
    t = tnew,
    itel = itel
  ))
}
```

runPenalty.R

```
runPenalty <-
  function(w,
           delta,
           lbd,
           p = 2,
           itmax = 10000,
           eps = 1e-10,
```

```
          cut = 1e-8,
          write = TRUE,
          verbose = FALSE) {
  m <- length(lbd)
  hList <- as.list(1:m)
  hList[[1]] <-
    smacofPenalty(
      w,
      delta,
      p,
      lbd = lbd[1],
      itmax = itmax,
      eps = eps,
      verbose = verbose
    )
  for (j in 2:m) {
    hList[[j]] <-
      smacofPenalty(
        w,
        delta,
        p,
        zold = hList[[j - 1]]$z,
        lbd = lbd[j],
        itmax = itmax,
        eps = eps,
        verbose = verbose
      )
  }
  mm <- m
  for (i in 1:m) {
    if (write) {
      cat(
        "itel",
        formatC(hList[[i]]$itel, width = 4, format = "d"),
        "lambda",
        formatC(
          hList[[i]]$l,
          width = 10,
          digits = 6,
          format = "f"
        ),
        "stress",
        formatC(
          hList[[i]]$s,
```

```
            width = 8,
            digits = 6,
            format = "f"
          ),
          "penalty",
          formatC(
            hList[[i]]$t,
            width = 8,
            digits = 6,
            format = "f"
          ),
          "\n"
        )
      }
      if (hList[[i]]$t < cut) {
        mm <- i
        break
      }
    }
    return(hList[1:mm])
  }

writeSelected <- function(hList, ind) {
  m <- length(hList)
  n <- length(ind)
  mn <- sort(union(union(1:3, ind), m - (2:0)))
  for (i in mn) {
    if (i > m) {
      next
    }
    cat(
      "itel",
      formatC(hList[[i]]$itel, width = 4, format = "d"),
      "lambda",
      formatC(
        hList[[i]]$l,
        width = 10,
        digits = 6,
        format = "f"
      ),
      "stress",
      formatC(
        hList[[i]]$s,
        width = 8,
```

```r
        digits = 6,
        format = "f"
      ),
      "penalty",
      formatC(
        hList[[i]]$t,
        width = 8,
        digits = 6,
        format = "f"
      ),
      "\n"
    )
  }
}
```

matchMe.R

```r
matchMe <- function (x,
                     itmax = 100,
                     eps = 1e-10,
                     verbose = FALSE) {
  m <- length (x)
  y <- sumList (x) / m
  itel <- 1
  fold <- sum (sapply (x, function (z)
    (z - y) ^ 2))
  repeat {
    for (j in 1:m) {
      u <- crossprod (x[[j]], y)
      s <- svd (u)
      r <- tcrossprod (s$u, s$v)
      x[[j]] <- x[[j]] %*% r
    }
    y <- sumList (x) / m
    fnew <- sum (sapply (x, function (z)
      (z - y) ^ 2))
    if (verbose) {

    }
    if (((fold - fnew) < eps) || (itel == itmax))
      break
    itel <- itel + 1
    fold <- fnew
  }
```

```r
  return (x)
}

sumList <- function (x) {
  m <- length (x)
  y <- x[[1]]
  for (j in 2:m) {
    y <- y + x[[j]]
  }
  return (y)
}
```

plotMe.R

```r
plotMe2 <- function(hList, labels, s = 1, t = 2) {
  n <- nrow(hList[[1]]$x)
  m <- length (hList)
  par(pty = "s")
  hMatch <- matchMe(lapply (hList, function(r)
    r$x))
  hMat <- matrix(0, 0, 2)
  for (j in 1:m) {
    hMat <- rbind(hMat, hMatch[[j]][, c(s, t)])
  }
  plot(
    hMat,
    xlab = "dim 1",
    ylab = "dim 2",
    col = c(rep("RED", n * (m - 1)), rep("BLUE", n)),
    cex = c(rep(1, n * (m - 1)), rep(2, n))
  )
  for (i in 1:n) {
    hLine <- matrix(0, 0, 2)
    for (j in 1:m) {
      hLine <- rbind(hLine, hMatch[[j]][i, c(s, t)])
    }
    lines(hLine)
  }
  text(hMatch[[m]], labels, cex = .75)
}

plotMe1 <- function(hList, labels) {
  n <- length(hList[[1]]$x)
```

```
  m <- length(hList)
  blow <- function(x) {
    n <- length(x)
    return(matrix(c(1:n, x), n, 2))
  }
  hMat <- matrix(0, 0, 2)
  for (j in 1:m) {
    hMat <- rbind(hMat, blow(hList[[j]]$x))
  }
  plot(
    hMat,
    xlab = "index",
    ylab = "x",
    col = c(rep("RED", n * (m - 1)), rep("BLUE", n)),
    cex = c(rep(1, n * (m - 1)), rep(2, n))
  )
  for (i in 1:n) {
    hLine <- matrix(0, 0, 2)
    for (j in 1:m) {
      hLine <- rbind(hLine, blow(hList[[j]]$x)[i,])
      lines(hLine)
    }
  }
  text(blow(hList[[m]]$x), labels, cex = 1.00)
  for (i in 1:n) {
    abline(h = hList[[m]]$x[i])
  }
}
```

checkUni.R

```
checkUni <- function (w, delta, x) {
  x <- drop (x)
  n <- length (x)
  vinv <- solve (smacofVmat (w) + (1 / n)) - (1 / n)
  return (drop (vinv %*% rowSums (w * delta * sign (outer (x, x, "-")))))
}
```

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