Smacof at 50: A Manual
Part 3
smacofAC: Additive Constant

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com/deleeuw in the smacofAC directories of the repositories smacofCode, smacofManual, and smacofExamples.

1 Introduction

In this part of the manual we discuss metric MDS, and the program smacofAC. Metric MDS is the core of all smacof programs, because they all have the majorization algorithm based on the Guttman transform in common.

There are two options, *bounds* and *constant*, to make smacofAC more widely applicable. Using these options the metric MDS problem becomes minimization of

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

over both X and $\hat{D}$, allowing some limited "metric" transformations of the data Δ. Here Δ^- and Δ^+ are known matrices with bounds, and c is an unknown additive constant. The four "metric" types of transformations relating disparities $\hat{d}_{ij}$ to dissimilarities δ_{ij} are

1. type AC1: if bounds = 0 and constant = 0 $\hat{d}_{ij} = \delta_{ij}$.
2. type AC2: if bounds = 0 and constant = 1 $\hat{d}_{ij} = \delta_{ij} + c$ for some c,
3. type AC3: if bounds = 1 and constant = 0 $\delta^-_{ij} \leq \hat{d}_{ij} \leq \delta^+_{ij}$,
4. type AC4: if bounds = 1 and constant = 1 $\delta^-_{ij} + c \leq \hat{d}_{ij} \leq \delta^+_{ij} + c$ for some c,

All four types of transformations also require that $\hat{d}_{ij} \geq 0$ for all (i, j). There are extensions of the smacof theory (Heiser (1991)) that do not require non-negativity of the disparities, but in the implementations in this manual we always force them to be non-negative. Note that AC3 is AC4 with $c = 0$ and AC2 is AC4 with $\Delta^- = \Delta^+ = \Delta$.

Note that for types AC2 and AC4 the data Δ do not need to be non-negative. In fact, the original motivation for the additive constant in classical scaling (Messick and Abelson (1956)) was that Thurstonian analysis of tetrad or triad comparisons produced dissimilarities on an interval scale, and thus could very well include negative values.

In AC3 and AC4 there is no mention of Δ, which means the bounds Δ^- and Δ^+ are actually the data. There are several possible uses of the bounds. We could collect dissimilarity data by asking subjects for interval judgments. Instead of a rating scale with possible responses from one to ten we could ask for a mark on a line between zero and ten, and then interpret the marks as a choice of one of the intervals $[k, k+1]$. These finite precision or interval type of data could even come from physical measurements of distances. Thus the bounds parameter provides one way to incorporate uncertainty into MDS, similar to interval analysis, fuzzy computing, or soft computing.

The non-negativity requirement for $\widehat{D}$ implies bounds for the additive constant c. In AC2 we need $c \geq -\min \delta_{ij}$ to maintain non-negativity. For AC4 we must have $c \geq -\min \delta_{ij}^+$, otherwise the constraints on the transformation are inconsistent. Clearly for consistency of AC3 and AC4 we require that $\delta_{ij}^- \leq \delta_{ij}^+$ for all (i, j). It makes sense in most situations to choose Δ^- and Δ^+ to be monotone with Δ, but there is no requirement to do so.

2 Program

2.1 Parameters

```
smacofAC <- function(delta,
                     ndim = 2,
                     wmat = NULL,
                     xold = NULL,
                     bounds = FALSE,
                     constant = FALSE,
                     deltalw = NULL,
                     deltaup = NULL,
                     alpha = 2,
                     labels = row.names(delta),
                     width = 15,
                     precision = 10,
                     itmax = 1000,
                     eps = 1e-10,
                     verbose = TRUE,
                     kitmax = 5,
                     keps = 1e-10,
                     kverbose = FALSE,
                     init = 1)
```

The parameters *constant*, *bounds*, *alpha*, *kitmax*, *kepsi*, and *kverbose* are only relevant for AC2, AC3, and AC4. Nevertheless even for AC1 they should have integer values, it just doesn't matter what these values are. Parameter *ndim* is the number of dimensions, and *init* tells if an initial configuration is read from a file (init = 1), is computed using classical scaling (init = 2), or is a random configuration (init = 3). Parameters *itmax*, *epsi*, and *verbose* control the iterations. The maximum number of iterations is *itmax*, the iterations stop if the decrease of stress in an iteration is less than 1E-*epsi*, and if *verbose* is one intermediate iteration results are written to stdout. These intermediate iteration results are formatted with the R function formatC(), using *width* for the width argument and *precision* for the digits argument.

2.2 Algorithm

2.2.1 Type AC1

This is standard non-metric smacof, no bells and whistles.

2.2.2 Type AC2

For AC2 we also optimize over the additive constant c, and thus the ALS algorithm has two sub-steps. The first sub-step consists of a number of Guttman iterations to update X for given $\widehat{D}$ (i.e. for given c) and the second sub-step updates c for given X. Parameters *kitmax*, *kepsi*, and *kverbose* control the inner iterations in the first sub-step in the same way as *itmax*, *epsi*, and *verbose* control the outer iterations that include both sub-steps. No inner iterations are used to update the additive constant, which only requires computing a weighted average.

$$c = -\frac{\sum\sum w_{ij}(\delta_{ij} - d_{ij}(X))}{\sum\sum w_{ij}}(\#eq:updac2) \tag{2}$$

AC2 should give the same results as the MDS method of Cooper (1972).

2.2.3 Type AC3

The algorithm for AC3 has the same structure as that for AC2. Instead of a second sub-step computing the additive constant, the second sub-step computes $\widehat{D}$ by squeezing the $D(X)$ into the bounds. Thus

$$\hat{d}_{ij} = \begin{cases} \delta_{ij}^- & \text{if } d_{ij}(X) < \delta_{ij}^-, \\ \delta_{ij}^+ & \text{if } d_{ij}(X) > \delta_{ij}^+, (\#eq:updac3) \\ d_{ij}(X) & \text{otherwise .} \end{cases} \tag{3}$$

Obviously no iterations are required in the second sub-step.

2.2.4 Type AC4

Of the four regression problems in the second ALS sub-step only the one for AC4 with both bounds and additive constant is non-trivial. We'll give it some extra attention.

It may help to give an example of what it actually requires. We use the De Gruijter example with nine Dutch political parties from 1967 (De Gruijter (1967)). For ease of reference we include the data here. Dissimilarities are averages over a group of 100 students from an introductory psychology course.

```
      KVP PvdA  VVD  ARP  CHU  CPN  PSP   BP  D66
KVP  0.00 5.63 5.27 4.60 4.80 7.54 6.73 7.18 6.17
PvdA 5.63 0.00 6.72 5.64 6.22 5.12 4.59 7.22 5.47
VVD  5.27 6.72 0.00 5.46 4.97 8.13 7.55 6.90 4.67
ARP  4.60 5.64 5.46 0.00 3.20 7.84 6.73 7.28 6.13
CHU  4.80 6.22 4.97 3.20 0.00 7.80 7.08 6.96 6.04
CPN  7.54 5.12 8.13 7.84 7.80 0.00 4.08 6.34 7.42
PSP  6.73 4.59 7.55 6.73 7.08 4.08 0.00 6.88 6.36
BP   7.18 7.22 6.90 7.28 6.96 6.34 6.88 0.00 7.36
D66  6.17 5.47 4.67 6.13 6.04 7.42 6.36 7.36 0.00
```

We compute distances from the Torgerson solution. The Shepard plot for $c = 0$ and the Torgerson distances is in figure @ref(fig:bandplot). The two blue lines are connecting the δ_{ij}^- and the δ_{ij}^+, i.e. they give the bounds for $c = 0$. In our example the lines are parallel, because $\delta_{ij}^+ - \delta_{ij}^- = 2$ for all (i, j), but in general this may not be the case. The points between the two lines do not contribute to the loss, and the points outside the band contribute by how much they are outside, as indicated by the black vertical fitlines.

By varying c we shift the region between the two parallel lines upwards or downwards. The width of the region, or more generally the shape, always remains the same, because it is determined by the difference of δ^+ and δ^- and does not depend on c. The optimal c is that shift for which the red $(\delta_{ij}, d_{ij}(X))$ points are as much as possible within the strip between the δ^- and δ^+ lines. This is in the least squares sense, which means that we minimize the horizontal squared distances from the points outside the strip to the δ^- and δ^+ lines (i.e. the black vertical lines).

Let's formalize this. Define

$$\phi_{ij}(c) := \min_{\delta_{ij} \geq 0} \{(\delta_{ij} - d_{ij}(X))^2 \mid \delta_{ij}^- + c \leq \delta_{ij} \leq \delta_{ij}^+ + c\}(\#eq:phiijdef) \tag{4}$$

and

$$\phi(c) := \sum\sum w_{ij}\phi_{ij}(c)(\#eq:phidef) \tag{5}$$

The constraints are consistent if $\delta_{ij}^{+} + c \geq 0$, i.e. if $c \geq c_0 := -\min \delta_{ij}^{+}$. The regression problem is to minimize ϕ over $c \geq c_0 := -\min \delta_{ij}^{+}$.

Figure has an example of one of the ϕ_{ij}. The value of the $d_{ij}(X)$ we used is , δ_{ij} is , δ_{ij}^{-} is , and δ_{ij}^{+} is . The two red vertical lines are at $c = d_{ij}(X) - \delta_{ij}^{+}$ and $c = d_{ij}(X) - \delta_{ij}^{-}$.

Now

$$\hat{d}_{ij} = \begin{cases} \delta_{ij}^{-} + c & \text{if } c \geq d_{ij}(X) - \delta_{ij}^{-}, \\ \delta_{ij}^{+} + c & \text{if } c \leq d_{ij}(X) - \delta_{ij}^{+}, (\#eq:solves) \\ d_{ij}(X) & \text{otherwise.} \end{cases} \tag{6}$$

and thus

$$\phi_{ij}(c) = \begin{cases} (d_{ij}(X) - (\delta_{ij}^{-} + c))^2 & \text{if } c \geq d_{ij}(X) - \delta_{ij}^{-}, \\ (d_{ij}(X) - (\delta_{ij}^{+} + c))^2 & \text{if } c \leq d_{ij}(X) - \delta_{ij}^{+}, (\#eq:funcs) \\ 0 & \text{otherwise.} \end{cases} \tag{7}$$

It follows that ϕ_{ij} is piecewise quadratic, convex, and continuously differentiable. The derivative is piecewise linear, continuous, and increasing. In fact

$$\mathcal{D}\phi_{ij}(c) = \begin{cases} 2(c - (d_{ij}(X) - \delta_{ij}^{-})) & \text{if } c \geq d_{ij}(X) - \delta_{ij}^{-}, \\ 2(c - (d_{ij}(X) - \delta_{ij}^{+})) & \text{if } c \leq d_{ij}(X) - \delta_{ij}^{+}, (\#eq:derivs) \\ 0 & \text{otherwise.} \end{cases} \tag{8}$$

Since ϕ is a positive linear combination of the ϕ_{ij} it is also piecewise quadratic, convex, and continuously differentiable, with a continuous piecewise linear increasing derivative. Note ϕ is **not** twice-differentiable and **not** strictly convex. Figure @ref(fig:morefunc) has a plot of ϕ for the De Gruijter example. The red vertical lines are at $c = c_0$ and at $c_1 := \max\{d_{ij}(X) - \delta_{ij}^{-}\}$. From @ref(eq:derivs) we see that if $c \geq c_1$ then $\mathcal{D}\phi(c_1) \geq 0$ and thus we can look for the optimum c in the interval $[c_0, c_1]$.

We minimize ϕ by using the R function optimize().

2.3 Output

2.4 Plots

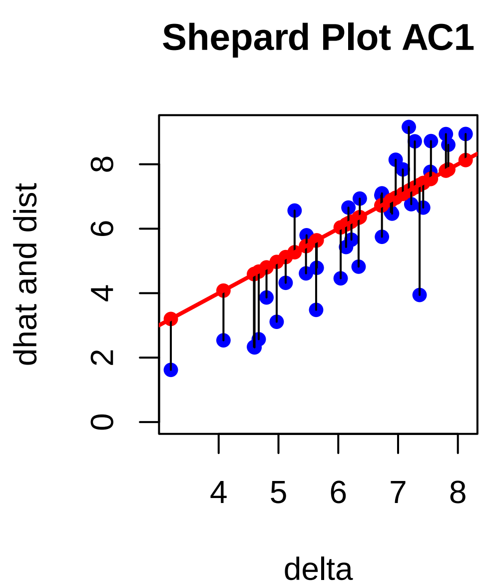
3 Examples

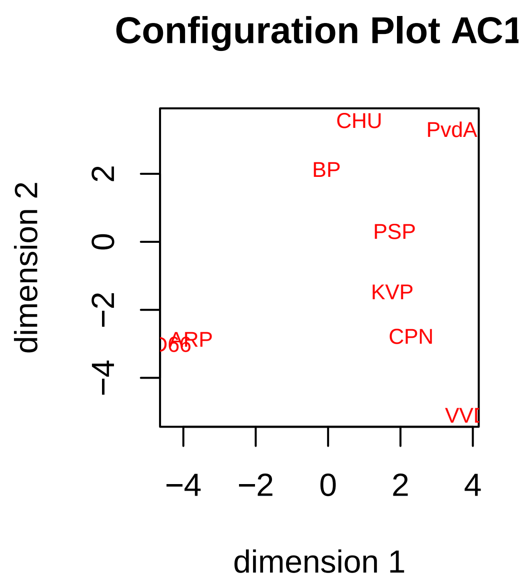
3.1 De Gruijter (1967)

It may help to give an example of what it actually requires. We use the De Gruijter example with nine Dutch political parties from 1967 (De Gruijter (1967)). Dissimilarities are averages over a group of 100 students from an introductory psychology course.

We compute optimal solutions for all four types AC1-AC4 (two dimensions, Torgerson initial estimate, no weights). We iterate until the difference in consecutive stress values is less than 1e-10. For each of the four runs we give the number of iterations, the final stress, and the additive constant in case of AC2 and AC4. We also make three plots: the Shepard plot with points $(\delta_{ij}, d_{ij}(X))$ in blue and with points $(\delta_{ij}, \hat{d}_{ij})$ in red, the configuration plot with a labeled X, and the dist-dhat plot with points $(d_{ij}(X), \hat{d}_{ij})$ scattered around the line $d = \hat{d}$. Line segments are drawn in the plots to show the fit of all pairs (i, j).

3.2 Type AC1

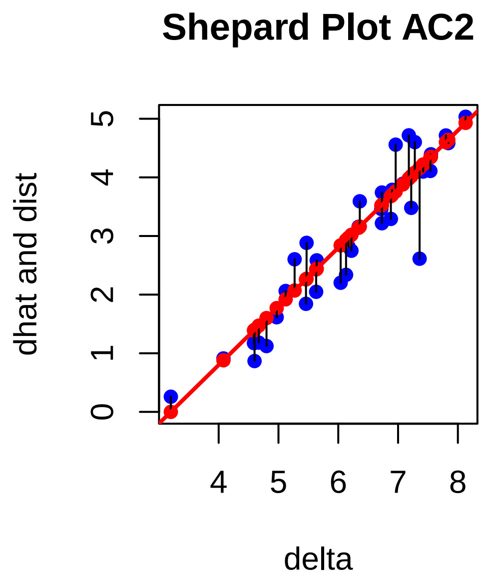


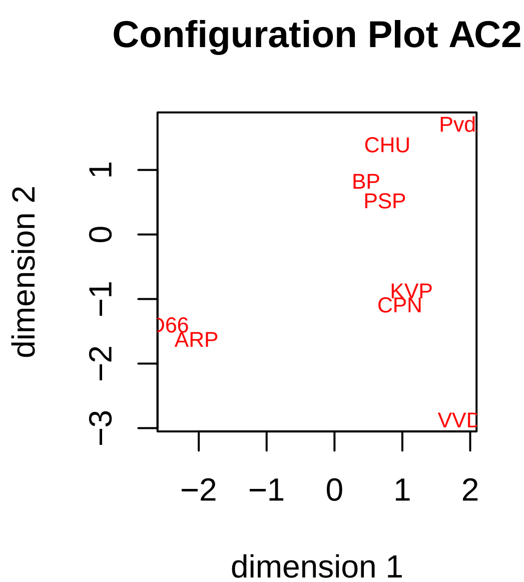


For AC1 we find a minimum stress of 32.2208145 after 112 iterations. The Shepard plot has a substantial intercept, which suggest that an additive constant may improve the fit. This is typical for average similarity judgments over heterogeneous groups of individuals. It is the reason why Ekman (1954) linearly transformed his average similarities so that the smallest became zero and the largest became one. That amounts to applying the additive constant before the MDS analysis.

To give some content to the configuration plot: CPN (communists), PSP (pacifists), and PvdA (social democrats) are leftists parties, ARP (protestants), CHU (other protestants), KVP (catholics) are religious parties, BP (farmers) is a right-wing protest party, VVD (classical liberals) is a conservative party, and D'66 (pragmatists, centrists) was brand new in 1967 and was supposedly beyond left and right.

3.3 Type AC2





As expected, the additive constant improves the fit. We have convergence after 25 iterations to stress 3.6661492. The additive constant is -3.2, which means the smallest $\delta_{ij} + c$, between ARP and CHU, is now zero. The configuration shows the same three groups, but they cluster a bit more tightly. This is to be expected. Without the additive constant the dissimilarities are more equal and consequently the distances are more equal to. The configuration tends more to what we see if all dissimilarities are equal, i.e. to points regularly spaced on a circle (De Leeuw and Stoop (1984)).

3.4 Type AC3

```
itel  1 sold    97.4130852810 smid   41.9550246691 snew     8.4543139218
itel  2 sold     8.4543139218 smid    7.4098292411 snew     6.6451369923
itel  3 sold     6.6451369923 smid    5.8490240542 snew     5.2489286201
itel  4 sold     5.2489286201 smid    4.6072125696 snew     4.1502164078
itel  5 sold     4.1502164078 smid    3.6168200275 snew     3.2322363271
itel  6 sold     3.2322363271 smid    2.7379930587 snew     2.4414269275
itel  7 sold     2.4414269275 smid    2.1593556178 snew     1.9752760141
itel  8 sold     1.9752760141 smid    1.8092882729 snew     1.6764432789
itel  9 sold     1.6764432789 smid    1.5582549338 snew     1.4557443279
itel  10 sold     1.4557443279 smid    1.3629036613 snew     1.2793695305
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itel  12 sold     1.1324574520 smid    1.0674066563 snew     1.0078467610
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```

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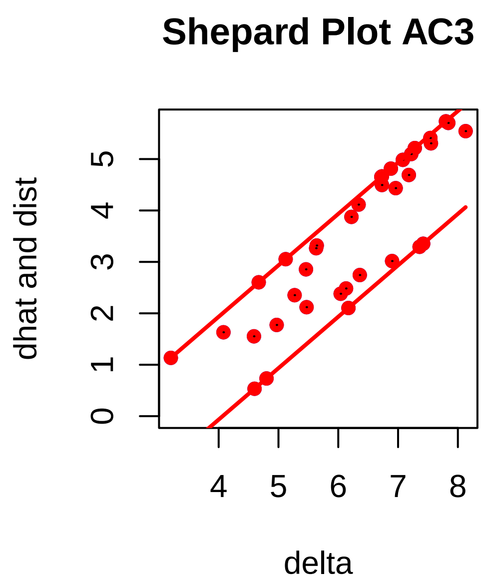
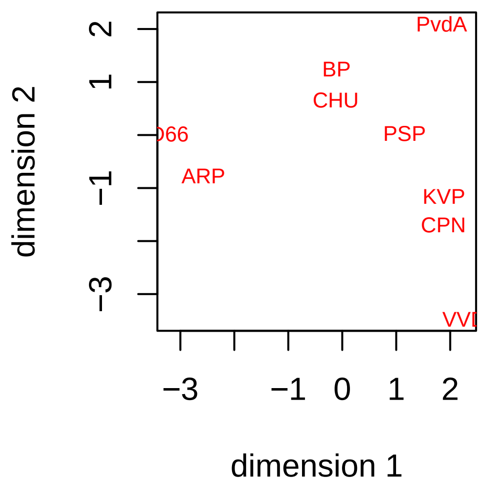
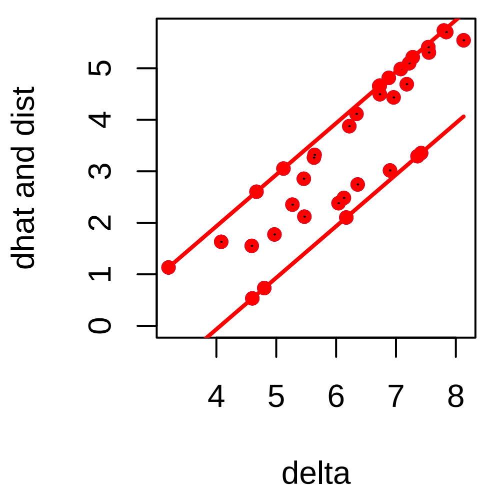


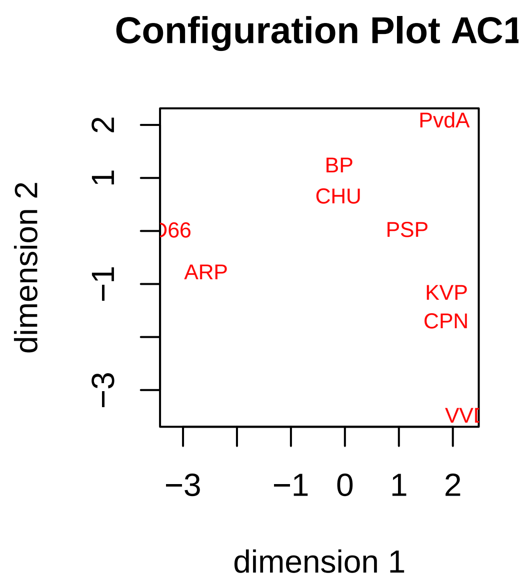
Configuration Plot AC3



The bounds we use are $\delta_{ij} \pm 1$. After 306 iterations we arrive at stress 2.3629831×10^{-8}. In the configuration plot the centrists have moved to the center. ## Type AC4

Shepard Plot AC1





After 306 iterations stress is 2.3629831×10^{-8}, i.e. practically zero. We succeeded in moving all distances within the bounds. The additive constant is -3.0664907. The configuration is again pretty much the same with D'66 in the center. VVD moves closer to the Christian Democrats, and BP is more isolated. # References

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