

# Smacof at 50: A Manual

## Part 2: smacofAC: Metric and Interval Smacof

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# 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

$$\sigma(X, \hat{D}) = \sum \sum w_{ij}(\hat{d}_{ij} - d_{ij}(X))^2 \quad (1)$$

over both  $X$  and  $\hat{D}$ , allowing some limited “metric” transformations of the data  $\Delta$ . Here  $\Delta^-$  and  $\Delta^+$  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  $\delta_{ij}$  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  $\Delta$  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  $\Delta$ , which means the bounds  $\Delta^-$  and  $\Delta^+$  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  $\hat{D}$  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  $\Delta^-$  and  $\Delta^+$  to be monotone with  $\Delta$ , 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  $\hat{D}$  (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.

$$c = -\frac{\sum \sum w_{ij}(\delta_{ij} - d_{ij}(X))}{\sum \sum w_{ij}} \quad (2)$$

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  $\hat{D}$  by squeezing the  $D(X)$  into the bounds. Thus

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

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 ???. The two blue lines are connecting the  $\delta_{ij}^-$  and the  $\delta_{ij}^+$ , 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  $\delta^+$  and  $\delta^-$  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  $\delta^-$  and  $\delta^+$  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  $\delta^-$  and  $\delta^+$  lines (i.e. the black vertical lines).

Let's formalize this. Define

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

and

$$\phi(c) := \sum \sum w_{ij} \phi_{ij}(c) \quad (5)$$

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  $\phi$  over  $c \geq c_0 := -\min \delta_{ij}^+$ .

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

Now

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

and thus

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

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

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

Since  $\phi$  is a positive linear combination of the  $\phi_{ij}$  it is also piecewise quadratic, convex, and continuously differentiable, with a continuous piecewise linear increasing derivative. Note  $\phi$  is **not** twice-differentiable and **not** strictly convex. Figure ?? has a plot of  $\phi$  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 (8) 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  $\phi$  by using the R function `optimize()`.

## 2.3 Output

## 2.4 Plots

# 3 Examples

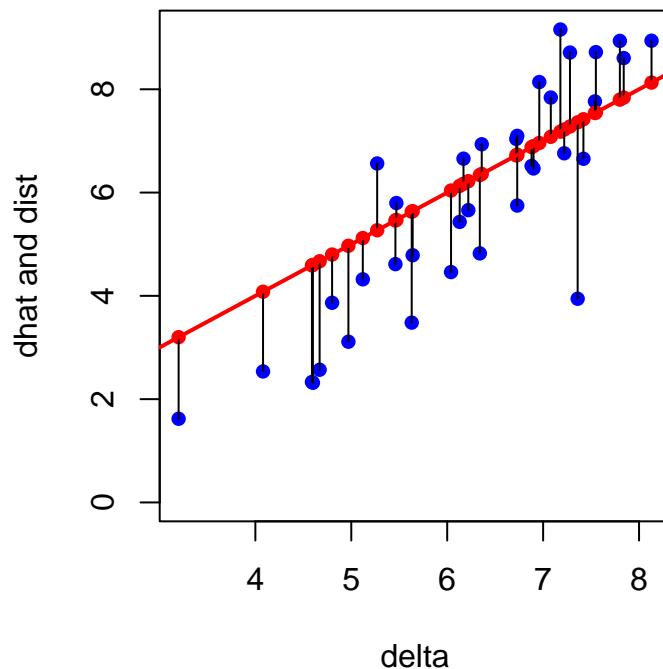
### 3.1 De Gruijter (1967)

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.

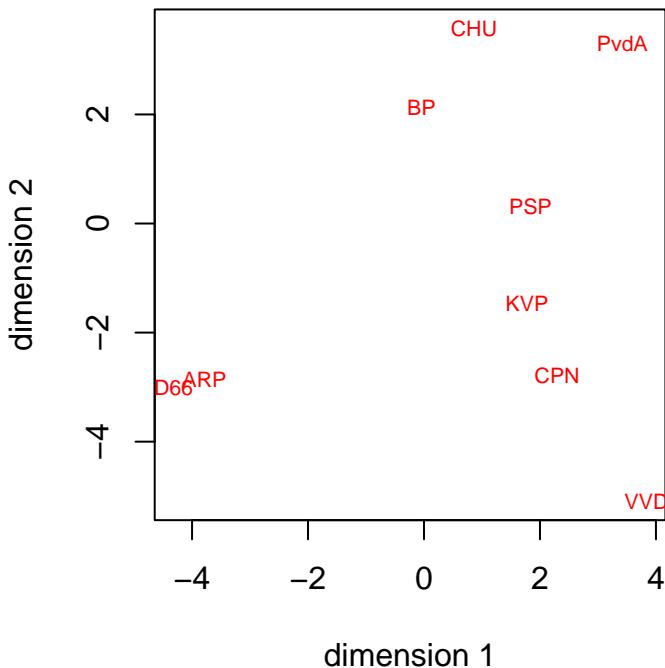
We compute optimal solutions for all four types AC1-AC4 (two dimensions, Torgerson initial estimate, no weights). We iterate until the difference in consecutive stress values is less than 1e-10. For each of the four runs we give the number of iterations, the final stress, and the additive constant in 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

**Shepard Plot AC1**



## Configuration Plot AC1

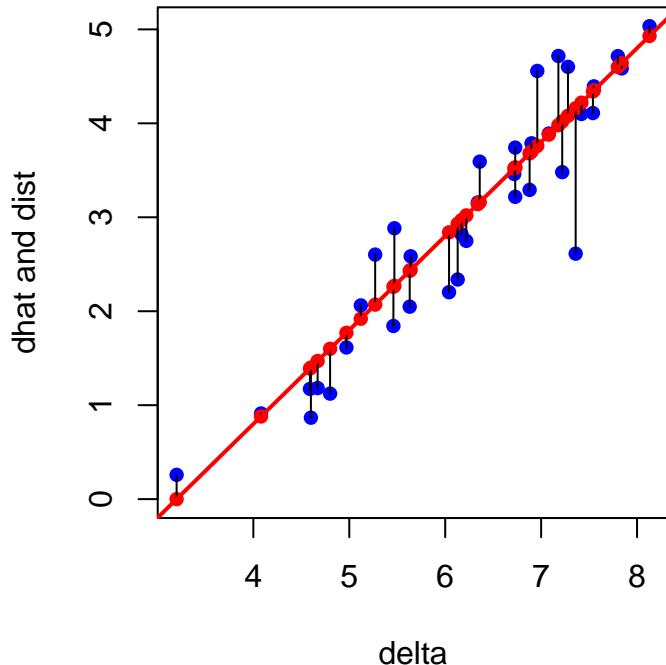


For AC1 we find a minimum stress of 32.2208145 after 112 iterations. The Shepard plot has a substantial intercept, which suggest that an additive constant may improve the fit. This is typical for average similarity judgments over heterogeneous groups of individuals. It is the reason why Ekman (1954) 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.

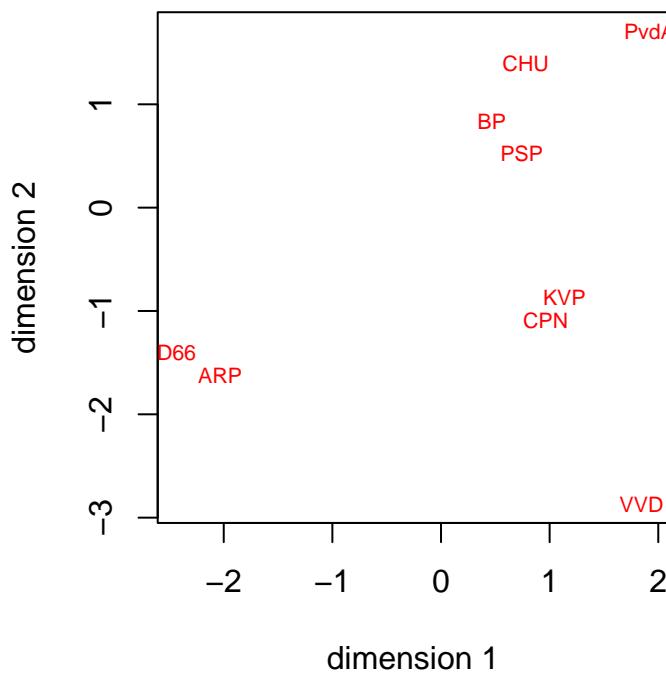
To give some content to the configuration plot: CPN (communists), PSP (pacifists), and PvdA (social democrats) are leftists parties, ARP (protestants), CHU (other protestants), KVP (catholics) are religious parties, BP (farmers) is a right-wing protest party, VVD (classical liberals) is a conservative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

### 3.3 Type AC2

**Shepard Plot AC2**



**Configuration Plot 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
## itel 11 sold	1.2793695305	smid	1.2025292754	snew	1.1324574520
## itel 12 sold	1.1324574520	smid	1.0674066563	snew	1.0078467610
## itel 13 sold	1.0078467610	smid	0.9522276636	snew	0.9013064460
## itel 14 sold	0.9013064460	smid	0.8535746120	snew	0.8098200136
## itel 15 sold	0.8098200136	smid	0.7685362919	snew	0.7305939018
## itel 16 sold	0.7305939018	smid	0.6945836967	snew	0.6615054424
## itel 17 sold	0.6615054424	smid	0.6300498204	snew	0.6011559114
## itel 18 sold	0.6011559114	smid	0.5735956560	snew	0.5483309878
## itel 19 sold	0.5483309878	smid	0.5241981027	snew	0.5020869304
## itel 20 sold	0.5020869304	smid	0.4809112562	snew	0.4614299495
## itel 21 sold	0.4614299495	smid	0.4425815492	snew	0.4251667367
## itel 22 sold	0.4251667367	smid	0.4082440772	snew	0.3925990995
## itel 23 sold	0.3925990995	smid	0.3773608282	snew	0.3632632528
## itel 24 sold	0.3632632528	smid	0.3494646668	snew	0.3366780605
## itel 25 sold	0.3366780605	smid	0.3241244799	snew	0.3124866156
## itel 26 sold	0.3124866156	smid	0.3010402505	snew	0.2904279430
## itel 27 sold	0.2904279430	smid	0.2799638410	snew	0.2702326078
## itel 28 sold	0.2702326078	smid	0.2606115288	snew	0.2516575222
## itel 29 sold	0.2516575222	smid	0.2427970344	snew	0.2345497021
## itel 30 sold	0.2345497021	smid	0.2263873344	snew	0.2187862641
## itel 31 sold	0.2187862641	smid	0.2112642137	snew	0.2042558938
## itel 32 sold	0.2042558938	smid	0.1973219792	snew	0.1908667641
## itel 33 sold	0.1908667641	smid	0.1844985022	snew	0.1785576365
## itel 34 sold	0.1785576365	smid	0.1726814275	snew	0.1672223800
## itel 35 sold	0.1672223800	smid	0.1618749397	snew	0.1568871640
## itel 36 sold	0.1568871640	smid	0.1520054971	snew	0.1474133814
## itel 37 sold	0.1474133814	smid	0.1429220273	snew	0.1386839988
## itel 38 sold	0.1386839988	smid	0.1345340757	snew	0.1306172696

## itel 39 sold	0.1306172696 smid	0.1267823207 snew	0.1231570280
## itel 40 sold	0.1231570280 smid	0.1195991686 snew	0.1162371624
## itel 41 sold	0.1162371624 smid	0.1129422950 snew	0.1098197491
## itel 42 sold	0.1098197491 smid	0.1067564820 snew	0.1038529288
## itel 43 sold	0.1038529288 smid	0.1009986094 snew	0.0982958229
## itel 44 sold	0.0982958229 smid	0.0956394236 snew	0.0931205429
## itel 45 sold	0.0931205429 smid	0.0906400571 snew	0.0882903384
## itel 46 sold	0.0882903384 smid	0.0859714475 snew	0.0837774185
## itel 47 sold	0.0837774185 smid	0.0816103623 snew	0.0795595988
## itel 48 sold	0.0795595988 smid	0.0775350522 snew	0.0756158480
## itel 49 sold	0.0756158480 smid	0.0737069060 snew	0.0718997892
## itel 50 sold	0.0718997892 smid	0.0700922565 snew	0.0683803581
## itel 51 sold	0.0683803581 smid	0.0666579412 snew	0.0650295657
## itel 52 sold	0.0650295657 smid	0.0633889911 snew	0.0618371988
## itel 53 sold	0.0618371988 smid	0.0602695635 snew	0.0587893711
## itel 54 sold	0.0587893711 smid	0.0572852862 snew	0.0558726314
## itel 55 sold	0.0558726314 smid	0.0544335762 snew	0.0530845479
## itel 56 sold	0.0530845479 smid	0.0517076720 snew	0.0504187686
## itel 57 sold	0.0504187686 smid	0.0490986716 snew	0.0478667578
## itel 58 sold	0.0478667578 smid	0.0466025175 snew	0.0454246636
## itel 59 sold	0.0454246636 smid	0.0442126511 snew	0.0430859071
## itel 60 sold	0.0430859071 smid	0.0419238186 snew	0.0408458015
## itel 61 sold	0.0408458015 smid	0.0397344293 snew	0.0387034342
## itel 62 sold	0.0387034342 smid	0.0376390715 snew	0.0366529538
## itel 63 sold	0.0366529538 smid	0.0356351002 snew	0.0346922685
## itel 64 sold	0.0346922685 smid	0.0337172756 snew	0.0328162870
## itel 65 sold	0.0328162870 smid	0.0318859969 snew	0.0310252529
## itel 66 sold	0.0310252529 smid	0.0301365454 snew	0.0293146845
## itel 67 sold	0.0293146845 smid	0.0284661882 snew	0.0276818686
## itel 68 sold	0.0276818686 smid	0.0268736638 snew	0.0261255295
## itel 69 sold	0.0261255295 smid	0.0253515999 snew	0.0246386243
## itel 70 sold	0.0246386243 smid	0.0239018541 snew	0.0232227235
## itel 71 sold	0.0232227235 smid	0.0225233461 snew	0.0218768243
## itel 72 sold	0.0218768243 smid	0.0212105688 snew	0.0205956586
## itel 73 sold	0.0205956586 smid	0.0199609330 snew	0.0193766033
## itel 74 sold	0.0193766033 smid	0.0187743001 snew	0.0182194345
## itel 75 sold	0.0182194345 smid	0.0176476992 snew	0.0171212966
## itel 76 sold	0.0171212966 smid	0.0165791103 snew	0.0160801664
## itel 77 sold	0.0160801664 smid	0.0155665396 snew	0.0150940641
## itel 78 sold	0.0150940641 smid	0.0146080603 snew	0.0141610730
## itel 79 sold	0.0141610730 smid	0.0137017748 snew	0.0132793044
## itel 80 sold	0.0132793044 smid	0.0128460418 snew	0.0124471117
## itel 81 sold	0.0124471117 smid	0.0120383862 snew	0.0116620659
## itel 82 sold	0.0116620659 smid	0.0112774626 snew	0.0109227851
## itel 83 sold	0.0109227851 smid	0.0105587161 snew	0.0102248820

## itel	84 sold	0.0102248820 smid	0.0098838778 snew	0.0095698425
## itel	85 sold	0.0095698425 smid	0.0092487574 snew	0.0089536963
## itel	86 sold	0.0089536963 smid	0.0086521341 snew	0.0083751510
## itel	87 sold	0.0083751510 smid	0.0080919781 snew	0.0078322169
## itel	88 sold	0.0078322169 smid	0.0075666147 snew	0.0073232264
## itel	89 sold	0.0073232264 smid	0.0070742856 snew	0.0068464430
## itel	90 sold	0.0068464430 smid	0.0066132474 snew	0.0064001456
## itel	91 sold	0.0064001456 smid	0.0061817952 snew	0.0059826528
## itel	92 sold	0.0059826528 smid	0.0057802663 snew	0.0055942116
## itel	93 sold	0.0055942116 smid	0.0054047931 snew	0.0052311501
## itel	94 sold	0.0052311501 smid	0.0050539660 snew	0.0048920336
## itel	95 sold	0.0048920336 smid	0.0047266122 snew	0.0045756432
## itel	96 sold	0.0045756432 smid	0.0044211081 snew	0.0042792136
## itel	97 sold	0.0042792136 smid	0.0041326493 snew	0.0039985613
## itel	98 sold	0.0039985613 smid	0.0038606482 snew	0.0037337299
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## itel	110 sold	0.0016446713 smid	0.0015838944 snew	0.0015303032
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## itel	119 sold	0.0009028660 smid	0.0008742102 snew	0.0008476717
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## itel	127 sold	0.0005501055 smid	0.0005331016 snew	0.0005171660
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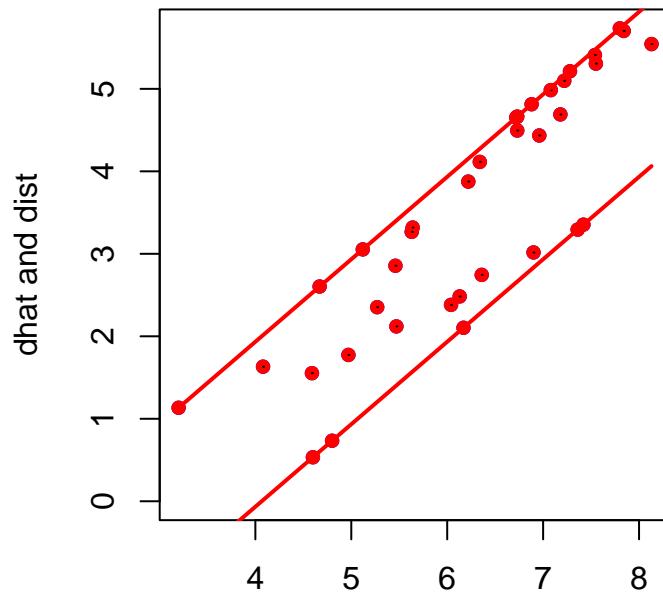
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## itel	193	sold	0.0000087061	smid	0.0000084327	snew	0.0000081715
## itel	194	sold	0.0000081715	smid	0.0000079148	snew	0.0000076696
## itel	195	sold	0.0000076696	smid	0.0000074285	snew	0.0000071984
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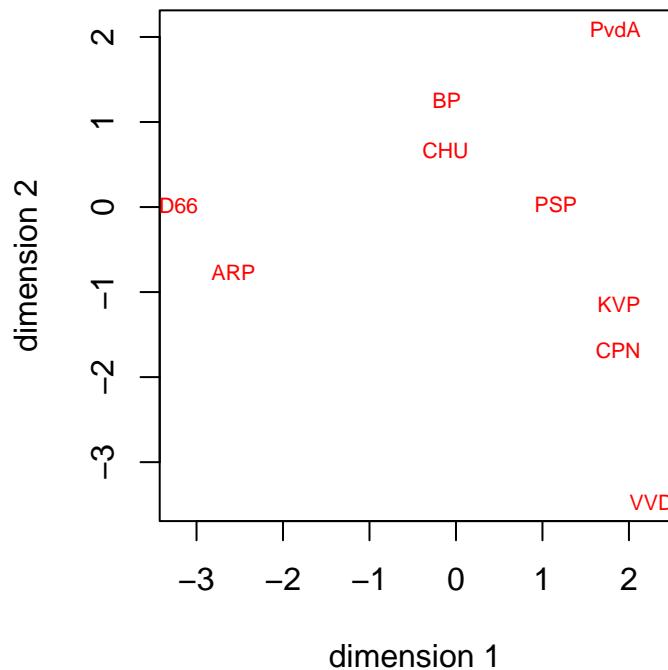
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## itel	274	sold	0.0000000577	smid	0.0000000565	snew	0.0000000550
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## itel	287	sold	0.0000000333	smid	0.0000000328	snew	0.0000000321
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## itel	291	sold	0.0000000290	smid	0.0000000286	snew	0.0000000281
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### Shepard Plot AC3

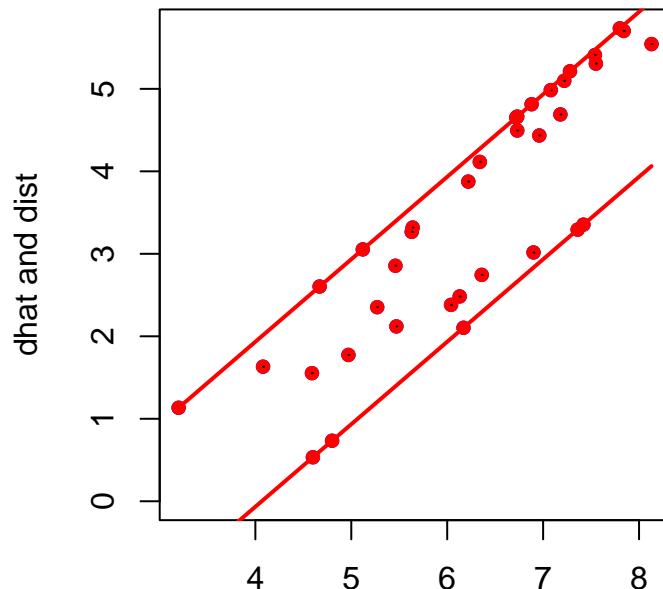


### Configuration Plot AC3

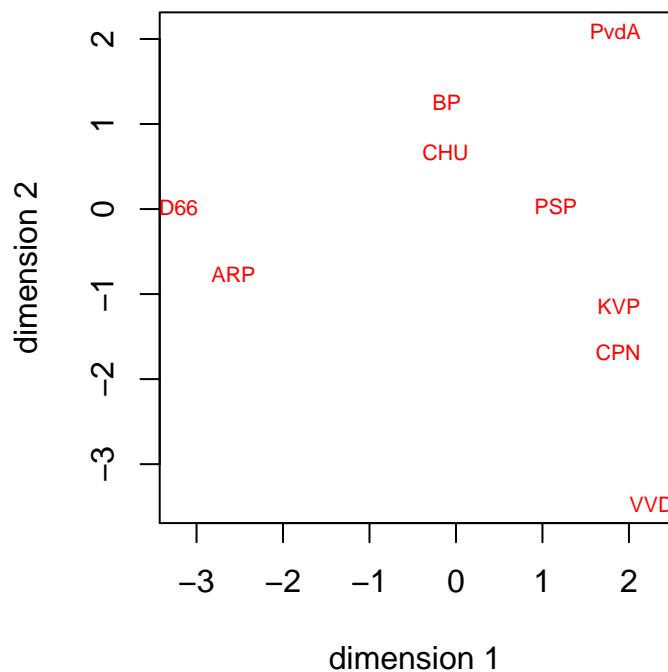


The bounds we use are  $\delta_{ij} \pm 1$ . After 306 iterations we arrive at stress  $2.3629831 \times 10^{-8}$ . In the configuration plot the centrists have moved to the center. ## Type AC4

### Shepard Plot AC1



### Configuration Plot AC1



After 306 iterations stress is  $2.3629831 \times 10^{-8}$ , 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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