

Part VI

Appendices

Appendix A

Computer Programs for MDS

Several computer programs for doing MDS exist, some of which are included in major software packages, and others are in the public domain. The list of programs we discuss in this appendix is not exhaustive, although we have tried to find the most important ones in terms of options and availability at the time of writing. Each program is described briefly. We also give an example of how a simple MDS job is run in each program. Where possible, we provide a subset of the commands and keywords needed for running a simple MDS analysis.

MDS is very much a visualization technique. Fortunately, the graphical capabilities of modern PCs have improved drastically over the years. Therefore, we place more emphasis on the graphical representations provided by MDS programs. In addition, we found two programs (GGVIS and PERMAP) freely available on the Internet that show interactively how the MDS solution is obtained. To reflect the development, we have organized the remainder of this appendix into three sections: the first section discusses two interactive MDS programs, the second section is focused mainly on commercial statistical packages that have high-resolution graphics, and the third section treats MDS programs that do not have high resolution graphics and have mostly been developed in the early days of MDS.

Table A.1 gives an overview of the properties of each of the programs. The MDS models in Table A.1 denote: (a) ordinal MDS with the primary approach to ties; (b) ordinal MDS with the secondary approach to ties; (c) ordinal MDS, using rank-image transformations; (d) interval MDS, $a + b \cdot p_{ij} = d_{ij}(\mathbf{X})$; (e) ratio MDS, $b \cdot p_{ij} = d_{ij}(\mathbf{X})$; (f) splines; (g) polynomial regression, $a + b \cdot p_{ij}(\mathbf{X}) + c \cdot p_{ij}^2(\mathbf{X}) + \dots = d_{ij}(\mathbf{X})$; (h) power, $p_{ij} = a \cdot d_{ij}^b(\mathbf{X})$,

which is equivalent to a linear MDS on logged proximities; (i) mixed models, for example, ordinal (unconditional) MDS for matrix 1 and linear MDS for a copy of matrix 1 stored in matrix 2. Note that (h) is but a linear MDS on logged proximities.

One general warning for the use of all programs is in place: many programs have rather weak convergence criteria, which may cause the program stopping the iterations too early and give suboptimal solutions. To be on the safe side, we advise to stop the iterative process only if the difference in two subsequent loss function values (usually Stress, or S-Stress) is smaller than 10^{-6} and setting the maximum number of iterations to 100 or more.

To illustrate the setup of a program, we use the artificial data on the ranking of pairs of politicians in Tables 9.4 and 9.3.

A.1 Interactive MDS Programs

With improving speed and graphical capabilities of modern computers, it becomes possible to animate the way in which MDS solutions are obtained. In this section, we discuss two of these programs, GGVIS and PERMAP. We call these programs an interactive form of MDS because they allow us to manipulate the MDS options by an easy user interface. Any change of MDS options usually leads to animations showing the changes leading to an optimal configuration. In such a way, you can test the stability of the solution interactively, for example, by eliminating points, changing the MDS model, rearranging points to check for local minima, and so on. These programs stay close to the exploratory nature of MDS with an emphasis on visualization.

GGVIS

GGVIS is a standard plug-in for MDS that comes with the GGOBI visualization software. It is freely available from the Internet and can be run as a standalone application or within the statistical programming environment R (also freely available). GGOBI visualizes rectangular two-way-two-mode data allowing an interactive grand tour through high-dimensional spaces, labeling, glyphing, connecting edges, and the like. GGVIS uses many of these options but is tailored for MDS. For an extensive discussion of GGVIS, we refer to Buja and Swayne (2002).

A nice feature of GGVIS is that a change of options has immediate effects on the solution. Thus, the user can see in real-time, for example, how the configuration changes from a metric to a nonmetric solution. Although the emphasis of GGVIS is on metric MDS, it also allows for ordinal transformations. Two options in GGVIS are unique. First, you can set interactively a power transformation of the dissimilarities and the resulting distribution is

TABLE A.1. A summary of several MDS programs; + stands for Yes or indicates that option is available, – shows that option is not available, n.a. means not applicable, and mem indicates that the maximum number of objects depends on memory available.

	GGVIS		Permap	Alscal	Newmdsx	Proxscal	SAS	Statistica	Systat	Fssa	Kyst	Minissa	Multiscale
<i>Platforms</i>													
Version	1.0.0b	11.3	n.a.	4.0.4	1.0	n.a.	4.5	11	3	2a	1	n.a.	
Standalone program	+	+	+	+	-	-	-	-	+	+	+	+	
In larger package	+	-	+	-	+	+	+	+	-	-	+	-	
Commercial	-	-	+	+	+	+	+	+	-	-	+	-	
MS-Windows	+	+	+	+	+	+	+	+	-	+	-	+	
Macintosh	-	-	+	-	+	+	+	+	-	+	-	+	
Graphical user interface	+	+	+	+	+	+	+	+	-	-	-	-	
High resolution graphics	+	+	+	+	+	+	+	+	-	-	-	-	
Dynamic graphics	+	+	-	-	-	-	-	-	-	-	-	-	
<i>General features</i>													
Minimizes Stress	+	+	-	+	+	+	+	+	-	+	+	+	
Minimizes S-Stress	-	+	+	-	-	+	-	+	-	-	-	-	
Minimizes alienation	-	-	-	+	-	-	-	+	+	-	+	-	
Maximizes likelihood	-	+	-	-	-	-	-	-	-	-	-	+	
Max. number of objects	mem	200	100	100	mem	mem	90	mem	50	60	100	mem	
Min. number of objects	2	2	4	2	2	2	2	2	3	3	2	3	
Max. dimensionality	<i>n</i> -1	4	6	10	<i>n</i> -1	<i>n</i> -1	9	5	10	6	10	<i>n</i> -1	
Processes rectangular data	+	+	+	+	+	-	-	+	-	+	+	+	
Allows for missing data	+	+	+	+	+	+	+	+	+	+	+	+	
Offers Minkowski distances	+	+	-	+	-	-	-	+	-	+	+	-	
Allows for weights w_{ij}	+	+	-	-	+	+	-	-	-	+	-	-	
<i>MDS models</i>													
Ordinal, prim. appr. ties	-	+	+	+	+	+	+	+	-	+	+	-	
Ordinal, sec. appr. ties	+	-	+	+	+	+	-	-	+	+	+	+	
Ordinal, rank-image	-	-	-	+	-	-	-	+	+	-	+	-	
Interval	-	+	+	-	+	+	-	+	-	+	-	+	
Ratio	+	+	+	-	+	+	-	-	-	+	-	+	
Absolute	+	-	+	-	-	+	-	-	-	-	-	+	
Splines	-	-	-	-	+	-	-	-	-	-	-	+	
Polynomial regression	-	-	+	-	+	-	-	-	-	+	-	+	
Power	-	-	-	-	+	-	-	+	-	-	-	-	
Mixed models	-	-	-	-	-	-	-	-	-	+	-	-	
<i>Special models</i>													
Split, by row	-	-	+	+	-	+	+	+	+	+	+	+	
Split, by row and by col.	-	-	-	+	-	-	-	-	-	+	+	-	
Split, by matrix	-	-	+	-	+	+	-	+	-	+	-	-	
Asymmetry models	-	-	+	-	-	-	-	-	-	-	-	-	
Weighted Euclidean model	-	-	+	+	+	+	-	+	-	-	+	+	
Generalized Euclidean model	-	-	+	+	+	-	-	-	-	-	+	-	
External variables	-	-	-	-	+	-	-	-	+	-	-	-	
Constrained solutions	-	+	+	+	+	+	-	-	-	+	+	-	



FIGURE A.1. Three different situations of the MDS settings windows of GGvis with four tabs at the top.

shown in a histogram. A power may be chosen such that the transformed dissimilarities have a uniform distribution (for an application, see Section 9.7). The second unique option is to set the weights that are applied to the errors to a power of the dissimilarities. Choosing a large positive power emphasizes the correct display of large dissimilarities, whereas a large negative power mostly ignores large dissimilarities and emphasizes the proper representation of small dissimilarities (see Section 11.3).

We tested a beta version of GGvis. To use GGvis, you first have to set up a data file that GGvis can process. Below, we present a sample file in XML. Once the data are read, move to the MDS module by choosing Tools > GGvis (MDS).... This brings up the window shown in Figure A.1.

Here, you can move to the fourth tab (or directly click on the “Run” button). It opens a window (see middle panel of Figure A.1) where you can change the default parameter settings for the dimensionality of the MDS space and the stepsize for the iterations. For our politicians data, we would set the dimensionality to 2, changing it from the default value of 3. To get an ordinal rather than a metric MDS solution, we would then press the pull-down menu “Metric MDS” in the middle of the window, where we can click on “Nonmetric MDS”. Then, click on the “Run MDS” button which starts the program showing how Stress is minimized and how the data are weighted (see windows in the middle of the right panel of Figure A.2). The ordinal MDS solution is given in Figure A.2.

The “Run MDS” button is a toggle. You may, for example, experiment with different stepsizes, metric vs. nonmetric MDS, different weights and so on, and rerun the MDS. From the “Reset” menu, you can reinitialize or

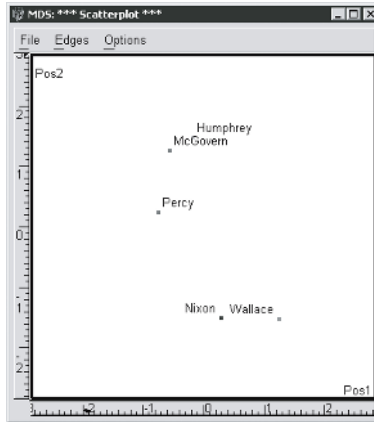


FIGURE A.2. Solution obtained by GGvis.

scramble the MDS configuration, and from the “View” menu you can view the Shepard diagram.

GGvis reads its data in XML format. Below you find an example. XML commands are written between `<>`-signs. Every command that is opened, for example, `<description>`, should also be closed again `</description>`. The first two lines define that these data belong to GGOBI.

```
<?xml version="1.0"?> <!DOCTYPE
ggobidata SYSTEM "ggobi.dtd">

<ggobidata count="2">
<data name="Politicians">
<description>
Example data set to illustrate {\sc Ggvis}
</description>
<variables count="0">
</variables>
<records count="5" glyph="fr 1" color="3">
<record id="1" label="Humphrey" color="1"> </record>
<record id="2" label="McGovern" color="3"> </record>
<record id="3" label="Percy" color="3"> </record>
<record id="4" label="Wallace" color="2"> </record>
<record id="5" label="Nixon" color="0"> </record>
</records>
</data>

<data name="dissimilarity">
<description>
Dissimilarities (rank orders)
</description>
<variables count="1">
<realvariable name="Dissimilarity" nickname="D" />
</variables>
<records count="10" glyph="fr 1" color="0">
```

```

<record source="1" destination="2"> 1 </record>
<record source="1" destination="3"> 5 </record>
<record source="1" destination="4"> 7 </record>
<record source="1" destination="5"> 6 </record>
<record source="2" destination="3"> 2 </record>
<record source="2" destination="4"> 10 </record>
<record source="2" destination="5"> 8 </record>
<record source="3" destination="4"> 9 </record>
<record source="3" destination="5"> 4 </record>
<record source="4" destination="5"> 3 </record>
</records>
</data>

</ggobidata>

```

GGVIS uses the following commands:

- `<ggobidata count="2">` says that what follows are two data sets specific for GGOBI.
- `<data name="Politicians">` specifies that the data defined here are called 'Politicians'.
- `<description>` allows a description of the data.
- `<variables count="0">` indicate that the rows defined below have no variables. If, for example, `count=1` then one lines should follow defining the variable name and nickname by `<realvariable name="Variable 1" nickname="V1" />`. For more variables, add more lines.
- `<records count="5" glyph="fr 1" color="3">` specifies that five records follow with a certain form of glyph type and color.
- `<record id="1" label="Humphrey" color="1"> </record>` defines the first record to have label 'Humphrey' and a specific color. If there is at least one variable, then their values should be specified before `</record>`.
- `<record source="1" destination="2"> 1 </record>` defines a single dissimilarity for objects 1 and 2. For all available dissimilarities, a single record should be specified indicating the row number and their column number. Missing dissimilarities are obtained by omitting the records for the missing pairs of objects.

More information can be found on the GGOBI website <http://www.ggobi.org>; E-mail: ggobi-help@ggobi.org

PERMAP

PERMAP is one of the few interactive MDS packages available. It allows users to interact directly with an MDS solution, move objects in the solution space, remove certain objects, and change MDS options. PERMAP is not built on any of the previously existing MDS software and can be freely downloaded from the Internet.

The program has a wide range of options, some of which are unique to PERMAP. It allows for ratio, interval, and ordinal MDS, the latter using the primary approach to ties. It can minimize several MDS loss functions,

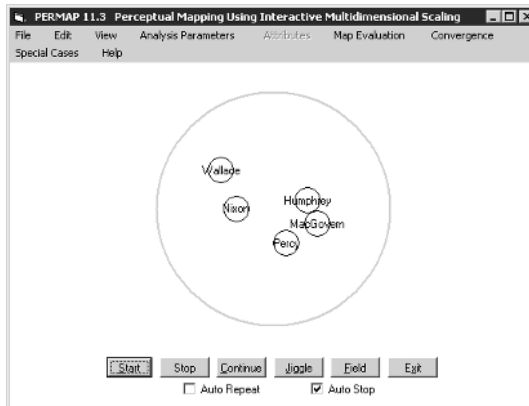


FIGURE A.3. Screen shot of PERMAP.

including Stress, Stress-1, S-Stress, and MULTISCALE. In addition, weights can be specified for every dissimilarity. PERMAP uses the general Minkowski distances that include Euclidean, city-block, and dominance distances. The program can also compute dissimilarities from a rectangular data matrix. A summary of the MDS solution can be saved into a text file. PERMAP comes with an extensive documentation aimed at the nonexpert.

A user-friendly option of PERMAP is to drag objects away from the solution into a “parking lot” to exclude the objects from the current MDS configuration. PERMAP will recompute the solution without these points. This option enables the user to test the influence of these points on the solution. If you want to use the object again, then you can drag the object back from the parking lot to the MDS configuration. In addition, points can be moved by dragging them around in the MDS solution. It is also possible to lock certain points that will keep them at a fixed location. Figure A.3 shows a screen shot of PERMAP using the politicians data. Text labels can be attached to the points by providing them as the first entry on a line with dissimilarities. The program can compute solutions in 1 to 4 dimensions. However, for three- or four-dimensional solutions, PERMAP shows a 2D projection of the 4D space. Note that these 2D projections may differ when PERMAP reruns the analysis.

The data input for PERMAP comes from a text file that can be written with any editor. The data file must be structured by certain specific keywords that instruct PERMAP how to read the information. Other text is simply ignored and can be used to explain the data. A simple setup for our politicians data looks like this:

```
TITLE= Example setup: politicians
NOBJECTS= 5
DISSIMILARITYLIST
Humphrey 0
MacGovern 1 0
```

Percy	5	2	0		
Wallace	7	10	9	0	
Nixon	6	8	4	3	0

A nonexhaustive list of subcommands of PERMAP is given below.

- **NOBJECTS** sets the number of objects.
- **TITLE** and **SUBTITLE** set the title and subtitle to be used in the output. If the **MESSAGE** and **SUBMESSAGE** are specified, then these are used in the output.
- **DISSIMILARITYLIST** or **SIMILARITYLIST** indicate that a triangular matrix with the dissimilarities or similarities are specified below. Note that the diagonal elements should be given as well and that NA specifies a missing value. If a dissimilarity line starts with a text entry, then it is used as a label for the points.
- **WEIGHTLIST** announces to PERMAP that the weights are specified below.
- **ATTRIBUTEList** specifies that the two-way data to be used to compute dissimilarities follow below. Note that **NATTRIBUTES** (indicating the number of columns of the two-way data) has to be defined before.
- **LOCATIONLIST** gives the initial configuration.
- **STARTMDSANALYSISType** defines the transformations. Choose 0 for a ratio transformation, 2 for interval, and 4 for ordinal primary approach to ties. The program cannot do the secondary approach to ties.
- **STARTBADNESSFUNCTION** defines what MDS loss function is used. Choose 0 for Stress, 1 for Stress-1, 2 for S-Stress, and 3 for MULTISCALE.
- **STARTDISTANCEFUNCTION** defines the distance to be used. Choose 0 for Euclidean distances, 1 for city-block, and 2 for Minkowski.
- **STARTATTRIBUTEFUNCTIONNUM** defines how the two-way data should be transformed into dissimilarities. Choose 0 for one minus the cosine of the angle between the vectors defined by the columns, 1 for Euclidean distances between the rows, 2 for city-block distances between the rows, 3 for one minus Guttman's μ_2 coefficient, 4 for the Pearson correlation between the columns, 5 for the Spearman rank correlation between the columns, 6 for the proportion of different categories between the rows (to be used for nominal variables). Options 7 to 12 are used for binary variables: 7 for the Jaccard indexes, 8 for Gower/Russel/Rao, 9 for Sokal-Michener distances, 10 for Hamman, 11 for Yule, and 12 for Askin/Charles.
- **STARTDIMENSIONNUM** allows to specify the dimensionality of the solution between 1 and 4.

Apart from the **NOBJECTS** command and a command to read the data, all other commands are optional.

For more information, contact Ron B. Heady, University of Louisiana at Lafayette, U.S.A. E-mail: ron@heady.us; Internet: <http://www.ucs.louisiana.edu/~rbh8900>

A.2 MDS Programs with High-Resolution Graphics

Current computers are able to provide high-resolution graphics, which is particularly important for a visualization technique such as MDS. All ma-

for statistical packages provide these high-resolution graphics. Below we discuss several MDS procedures available in commercial statistical packages and a package called NEWMDX[©] that provides a shell for text-based MDS programs that produce high-resolution graphics.

ALSCAL

ALSCAL (Takane et al., 1977) is one of the current MDS modules in SPSS. ALSCAL differs from other MDS programs in minimizing S-Stress rather than Stress, thereby fitting squared distances to squared dissimilarities. As a result, in ALSCAL the large dissimilarities are much better represented than the small dissimilarities. ALSCAL is a flexible MDS program that also provides models for asymmetric data, unfolding, and three-way analyses (by the weighted or generalized Euclidean model). Many options can be combined. ALSCAL also allows coordinates to be fixed, which is especially useful for external unfolding.

ALSCAL can be started in SPSS by choosing the menu “Analyze > Scale > Multidimensional Scaling...”. Using dialogue boxes, the ALSCAL options can be specified. In addition, (dis)similarity matrices can be created from rectangular data matrices. Alternatively, ALSCAL can be run through SPSS-syntax allowing for some more options. Some care has to be taken when adapting a configuration plot in ALSCAL. If you change the range of the axes or resize the plot differently for the two axes, then the horizontal units can be different from the vertical units so that the distances you see may be misleading. In addition, the default convergence criterion is far too weak and should be manually tightened to, say, .000001 or smaller.

A sample setup for an ordinal MDS analysis with ALSCAL of a 5×5 matrix of dissimilarity scores on five politicians is this:

```
TITLE 'Alscal in SPSS example setup: politicians'.
MATRIX DATA /VARIABLES Humphrey McGovern Percy Wallace Nixon
/CONTENTS PROX /FORMAT LOWER NODIAGONAL.
BEGIN DATA
1
5 2
7 10 9
6 8 4 3
END DATA.
ALSCAL /VARIABLES Humphrey McGovern Percy Wallace Nixon
/CRITERIA CONVERGE(0.000001) ITER(100) STRESSMIN(0.000001)
/LEVEL ORDINAL.
```

Commands in SPSS are ended by a dot (.); subcommands start with a slash (/) and usually have one or more keywords; keywords are printed in caps.

The ALSCAL job above first formulates a TITLE. It then defines the data setup in the MATRIX DATA command and lists the proximities between BEGIN DATA and END DATA. In the MATRIX DATA command, /VARIABLES should be followed by a list of variable names,

one for each variable (object, point). This list can also be abbreviated by 'VAR1 TO VAR5' or 'OBJECT1 TO OBJECT5'. The variable names are at most eight characters long. The subcommand /CONTENTS PROX indicates that the contents is a proximity matrix. /FORMAT LOWER NODIAGONAL indicates that only the lower triangular elements of the proximities are to be read. Finally, the desired MDS model is specified in the ALSICAL command: The VARIABLES option lists the variables that are to be mapped into points; the CRITERIA option specifies a number of technical requests for the optimization; the LEVEL option requests an ordinal MDS.

Some optional subcommands of ALSICAL are:

- /SHAPE specifies the shape of the dissimilarity matrix. Valid keywords are SYMMETRIC, ASYMMETRIC, and RECTANGULAR. SHAPE = RECTANGULAR defines unfolding.
- /LEVEL indicates the allowed transformation of the dissimilarities. Default is ORDINAL, which does monotone regression with the secondary approach to ties. For the primary approach specify, ORDINAL(UNTIE). If the proximities are similarities instead of dissimilarities, you can specify ORDINAL(SIMILAR), which may be combined with UNTIE. The keyword INTERVAL indicates interval transformations. For example, INTERVAL(3) specifies polynomial regression of the order 3. RATIO excludes the intercept and followed by '(2)' indicates quadratic polynomial regression.
- /CONDITION specifies conditionality of the transformations. In three-way scaling, MATRIX indicates that for each replication a separate transformation of the proximities has to be found (default). UNCONDITIONAL specifies that there is only one transformation for all replications. ROW means that the proximities in every row may have a different transformation, which is useful for unfolding.
- /MODEL indicates which model has to be used. EUCLIDEAN indicates the ordinary Euclidean distance (default), INDSCAL specifies the individual differences (weighted) Euclidean distance model.
- /CRITERIA controls the stopping conditions of the algorithm. CONVERGENCE (.000001) causes the program to stop whenever the difference in S-Stress between subsequent iterations is less than .000001. ITER(100) sets the maximum number of iterations to 100. STRESSMIN(.0001) causes the iterations to stop whenever S-Stress is less than .0001. NEGATIVE allows negative dimension weights in the INDSCAL model. CUTOFF(0) causes negative proximities to be treated as missing (default). DIMENS(2,5) causes ALSICAL to compute a solution in 5 dimensions, then 4, 3, and 2 dimensions. Default is DIMENS(2,2).
- /PRINT specifies print options. DATA prints the proximities. INTERMED prints intermediate results, which can generate a huge amount of output. HEADER prints a summary of options specified.
- /PLOT controls the plots made by ALSICAL. Defaults are the plots for the object configuration, the weight matrix (for INDSCAL) and Shepard plots. In addition, ALL generates a transformation plot for every replication or row (depending on CONDITION) and a plot of the weighted object coordinates for every replication (when appropriate).

For more information, contact: worldwide headquarters SPSS Inc. 233 S. Wacker Drive, 11th Floor, Chicago, IL 60606-6307, U.S.A. Phone: (312) 651-3000; Fax: (312) 651-3668; Internet: <http://www.spss.com>



FIGURE A.4. NEWMDSX[©] wizard for constructing MINISSA input.

	Stimulus 1	Stimulus 2	Stimulus 3	Stimulus 4
McGovern	1	#####	#####	#####
Percy	6	2	#####	#####
Wallace	2	10	9	#####
Nixon	6	8	4	3

FIGURE A.5. NEWMDSX[©] data entry window for MINISSA.

NEWMDSX[©]

Many of the first-generation MDS programs have text-based input and output, and no graphical user interface nor high-resolution graphics. The package NEWMDSX[©] is aimed to fill this gap. It offers a shell with an easy graphical user interface to run a variety of programs reported in the literature. In this shell, you can start a wizard to construct the input file for the program you want; see Figure A.4 (based on a beta version of NEWMDSX[©], version 4.0.4.). It also has several ways to read data, including a spreadsheet-like data entry window; see Figure A.5. The MDS program included in NEWMDSX[©] is MINISSA (discussed separately in Section A.3).

NEWMDSX[©] has high-resolution graphics for configurations in one to three dimensions. In addition, it provides Shepard diagrams and Stress plots. For hierarchical clustering it provides a dendrogram. The graphics the program produces can be edited.

In Figure A.6, an example is given of the graphics windows. NEWMDSX[©] is the only package currently available that provides a relatively easy interface for the MDS programs developed from 1960 to 1980. Table A.2 contains an overview of the MDS programs included, many of which are discussed in this book. NEWMDSX[©] is a package with not too many options but with a rich amount of MDS programs.

More info at: E-mail: enquiries@newmdsx.com; Internet: <http://www.newmdsx.com>

PROXSCAL

PROXSCAL is a program for least-squares MDS minimizing Stress available in SPSS (Commandeur & Heiser, 1993; Meulman, Heiser, & SPSS, 1999). It builds on the majorizing algorithm of De Leeuw and Heiser (1980) (see Chapter 8), which guarantees convergence of Stress. PROXSCAL offers a large variety of options for MDS analysis. One of the unique features of PROXSCAL is that the user can impose external constraints on the MDS

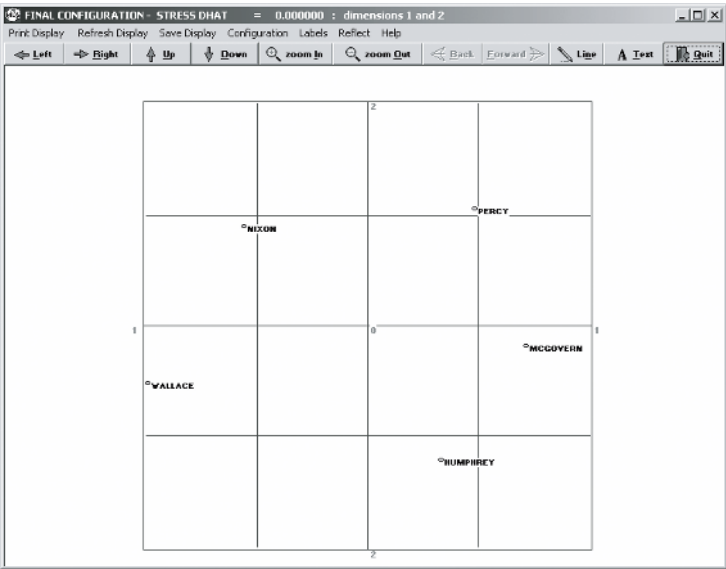


FIGURE A.6. Graphics window obtained by NEWMDSX[©].

TABLE A.2. Overview of programs that can be run within NEWMDSX[©].

Program	Remarks
CANDECOMP	Three-way decomposition for three-way data.
CONJOINT	Performs unidimensional conjoint analysis.
CORRESP	Correspondence analysis.
HICLUS	Performs hierarchical clustering on dissimilarity data using single or complete linkage.
INDSCAL-S	Individual Differences SCALing for fitting the weighted Euclidean distances.
MDSORT	MDS of sorting data.
MDPREF	MultiDimensional PREference for the vector model of unfolding.
MINI-RSA	Ideal point unfolding model.
MINISSA	Nonmetric MDS program.
MRSCAL	MetRic SCALing for metric MDS with Minkowski distances.
PARAMAP	For maximizing local monotonicity.
PINDIS	Procrustean Individual Differences Scaling for doing Procrustes analysis.
PREFMAP	PREference MAPping for external unfolding using the ideal point or vector model for unfolding.
PRO-FIT	PROperty FITting for external unfolding using the vector model.
TRISOSCAL	TRIadic Similarities Ordinal SCALing for MDS analysis of triadic dissimilarities.
WOMBATS	Work Out Measures Before Attempting To Scale converts a two-way two-mode data matrix into a dissimilarity matrix.

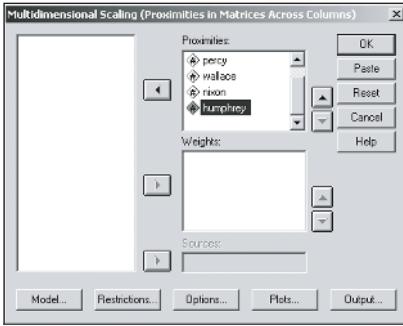


FIGURE A.7. Main dialogue boxes in SPSS PROXSCAL.

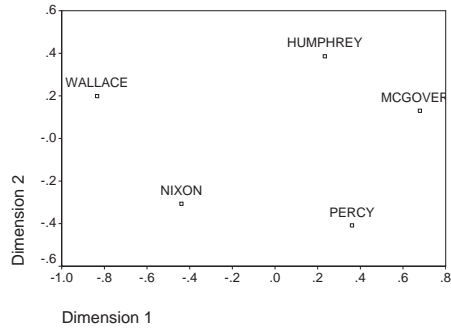


FIGURE A.8. PROXSCAL solution of the politicians data.

configuration, such as the restriction that the coordinates are a linear combination of some external variables (see Section 10.3). It also allows fixing some of the coordinates. These options can be combined with the weighted Euclidean model (Section 22.1) or the generalized Euclidean model (Section 22.2). The implementation of these models in PROXSCAL never gives negative dimension weights.

PROXSCAL can attach user-defined weights to every proximity. The transformations of the proximities in PROXSCAL are ordinal, interval, power, and monotone spline. PROXSCAL is the only program that avoids negative disparities that may arise when specifying an interval transformation of the dissimilarities as shown by Heiser (1990).

PROXSCAL can be specified in SPSS by choosing the menu “Analyze > Scale > Multidimensional Scaling (PROXSCAL)...”. The main dialogue box of PROXSCAL is given in Figure A.7. Most options can be accessed through dialogue boxes. However, some options can only be specified using syntax.

```
TITLE 'Proxscal in SPSS example setup: politicians'.
MATRIX DATA /VARIABLES Humphrey McGovern Percy Wallace Nixon
/CONTENTS MAT /FORMAT LOWER NODIAGONAL.
BEGIN DATA
1
5 2
7 10 9
6 8 4 3
END DATA.
PROXSCAL /VARIABLES Humphrey McGovern Percy Wallace Nixon
/SHAPE = LOWER
/INITIAL = TORGERSON
/CRITERIA = DIMENSION(2) DIFFSTRESS(0.000001)
MAXITER(100) MINSTRESS(0.000001)
/TRANSFORMATION = ORDINAL.
```

PROXSCAL has many different options, some of which are only accessible from syntax. The commands in the example above up to PROXSCAL correspond to those discussed

above for the ALSICAL program. A nonexhaustive list of subcommands of PROXSCAL is given below.

- `/VARIABLES` specifies the columns of the dissimilarity matrix. Unless the `/TABLE` subcommand is used, the number of rows should be a multiple of the number of variables specified. In the simple case of a single dissimilarity matrix, the number of rows is equal to the number of columns. For three-way analyses, the replications should be stacked underneath each other. The labels used in the plot are either the variable names or their variable labels.
- `/TABLE` allows to read dissimilarities from a single column. To identify a dissimilarity, two extra variables are needed: its row and column number. If three-way data are present, a third variable is needed to define the replication (called a source in PROXSCAL). The value labels to the row, column, and replication variable are used as labels in the plots.
- `/SHAPE` specifies the shape of the dissimilarity matrix. Valid keywords are `LOWER`, `UPPER`, and `BOTH` to specify respectively the lower part of the dissimilarity matrix, the upper part, or the symmetrized table.
- `/WEIGHTS` is used to specify nonnegative weights for weighting the residuals. The weights are read similarly as the dissimilarities as specified by the `VARIABLES` subcommand.
- `/PROXIMITIES` defines whether the data are assumed to be `DISSIMILARITIES` (default) or `SIMILARITIES`.
- `/INITIAL` specifies what initial configuration is used. `SIMPLEX` (default) uses a PROXSCAL specific start assuming that all objects are at distance one of each other. `TORGERSON` defines classical scaling as a start configuration. This option tends to give better quality solutions than `SIMPLEX`. `RANDOM(N)` computes a PROXSCAL solution for `n` random starts and reports the best.
- `/TRANSFORMATION` indicates the allowed proximities of the dissimilarities. Default is `RATIO` where the dissimilarities are only multiplied such that the disparities have a specific sum of squares. The keyword `INTERVAL` indicates interval transformations. `ORDINAL` does monotone regression with the secondary approach to ties and `ORDINAL(UNTIE)` specifies the primary approach to ties. `SPLINE(DEGREE,INKNOT)` specifies a spline transformation of order `degree` and `inknot` interior knots.
- `/CONDITION` specifies the conditionality of the transformations. In three-way scaling, `MATRIX` indicates that for each replication a separate transformation of the proximities has to be found (default). `UNCONDITIONAL` specifies that there is only one transformation for all replications.
- `/MODEL` has the `IDENTITY` model as default thereby modeling all replications by the same configuration. For three-way data, `WEIGHTED` indicates the weighted Euclidean distance so that dimensions may differ in the third way according to their individual dimension weight. `GENERALIZED` specifies the individual differences (weighted) Euclidean distance model. `REDUCED` specifies the reduced rank model.
- `/CRITERIA` controls the stopping conditions of the algorithm. `CONVERGENCE(.000001)` causes the program to stop whenever the difference in S-Stress between subsequent iterations is less than .000001. `MAXITER(100)` sets the maximum number of iterations to 100. `MINSTRESS(.0001)` causes the iterations to stop whenever Stress is less than .0001. In addition, by `DIMENSIONS(DMIN,DMAX)` you can let PROXSCAL compute solutions from `dmax` dimensions to `dmin` dimensions.
- `/PRINT` specifies print options. `INPUT` prints the proximities, `HISTORY` the history of iterations, `STRESS` several standard Stress measures, `DECOMPOSITION` a decomposition of Stress into Stress per object and possibly per replication, `COMMON` the

coordinates, DISTANCES the distances, WEIGHTS the weights used by the generalized or weighted Euclidean distances found by three-way models, and TRANSFORMATION the transformations.

- /PLOT controls the plots made by PROXSCAL. Defaults are the plots for the object configuration (COMMON), and the weight matrix (WEIGHTS) for three-way models. In addition, a STRESS-plot is available for plotting Stress against the number of dimensions of the solution, TRANSFORMATION for plotting the the data against the disparities, RESIDUALS for plotting the disparities against the distances, and INDIVIDUAL for plotting the coordinates of replications in three-way models. Note that PROXSCAL does not provide a Shepard plot.

For more information contact: Frank M.T.A. Busing, Dept. of Psychometrics, Univ. of Leiden, P.O. Box 9555, 2300 RB Leiden, The Netherlands. E-mail: busing@fsw.leidenuniv.nl; Internet: <http://www.spss.com>

SAS

SAS is a comprehensive system of software products for managing, analyzing, and presenting data. SAS has versions for virtually all platforms. SAS can be run in batch mode, submit mode, interactive line mode, and display manager (windows) mode. SAS used to offer ALSCAL as its MDS module but now has replaced ALSCAL by ‘PROC MDS’. This program has many options, some of them rather tricky ones, with effects that are difficult to predict.

In batch mode, our sample MDS job can be set up in the SAS command language as follows. SAS commands and options are printed in capital letters. Commands are ended with a ;.

```
DATA polit;
TITLE Politicians Example;
INPUT (var1-var5)(3.) @21 name $ 8.;
CARDS;
  0                Humphrey
  1  0                McGovern
  5  2  0                Percy
  7 10  9  0                Wallace
  6  8  4  3  0            Nixon
;
PROC MDS DIM=2 LEVEL=ORDINAL PFINAL PCONFIG OUT=OUT OUTRES=RES;
OBJECT name;
RUN;
```

The job first reads five numeric variables in fixed format (fields of length 3) and one alphanumeric variable, “name”, in a field of length 8, starting in column 21. Then, the MDS procedure is called, together with a set of options. PROC MDS analyzes the proximities among all variables at the ordinal measurement level (LEVEL=ORDINAL) in two dimensions (DIMENSION=2. The fit values and the configuration are printed (PFINAL and PCONFIG, respectively). The estimates and fitted values are saved in output data files

(“out” and “res”, respectively). PROC MDS produces no plots. For plotting, one must utilize special plotting procedures with the output files.

SAS has its own command language. The following summarizes the most important commands for PROC MDS. The general syntax is:

```
PROC MDS options;
  VAR variables;
  INVAR variables;
  OBJECT variable;
  SUBJECT variable;
  WEIGHT variable;
  BY variables;
```

The PROC MDS statement is required. All other statements are optional. The VAR statement defines the numeric variables in the file DATA = xyz that contain the proximities. Each variable corresponds to one object/point. If VAR is omitted, all numeric variables not specified in another statement are used. The INVAR statement defines the numeric variables in the file INITIAL=xyz, the initial configuration, where the first variable contains the coordinates on the first dimension, ..., the m th variable the coordinate on the m th dimension. The WEIGHT statement specifies a numeric variable in the file DATA=xyz that contains weights for each proximity. The number of WEIGHT variables must be the same as the number of VAR variables, and the variables in the WEIGHT statement must be in the same order as the corresponding variables in the VAR statement. If no WEIGHT statement is used, all data within a partition are assigned equal weight. The BY statement is used to obtain separate MDS analyses on groups of proximity data defined by the BY variables. The OBJECT statement defines a variable that contains descriptive labels for the points. The SUBJECT statement specifies a variable in the file DATA = xyz that contains descriptive labels for the data matrices or “subjects”.

The options for PROC MDS are:

- The Proximities
 - DATA = SAS file name, the data set containing one or more *square* matrices to be analyzed. (The requirement to input square proximity matrices makes the procedure clumsy for unfolding applications, because off-diagonal matrices cannot be processed directly. Rather, they have to be defined as submatrices within a square matrix with missing values.) Usually, there is one matrix per person. Data are generally assumed to be dissimilarities unless (a) there are diagonal elements that are generally larger than the off-diagonal elements or (b) one uses the SIMILAR option.
 - SIMILAR causes the data to be treated as similarities.
 - SHAPE = TRIANGULAR | SQUARE determines whether the entire data matrix for each subject is stored and analyzed or only one triangle of the matrix. Default is triangle, unless CONDITION = ROW.
- The MDS Model
 - LEVEL = ABSOLUTE | RATIO | INTERVAL | LOGINTERVAL | ORDINAL specifies the admissible transformation on the proximities.
 - CONDITION = UN | MATRIX | ROW. Conditionalities of proximities. Default is MATRIX.
 - DIMENSION = m_{\min} [TO m_{\max}], where $1 \leq m_{\min} \leq m_{\max} < n$. Skipping the TO term leads to $m_{\min} = m$.

- CUTOFF = k , causes data less than k to be treated as missing values. Default value is 0.
 - UNTIE specifies the primary approach to ties for LEVEL = ORDINAL.
 - NEGATIVE allows slopes or powers to be negative with LEVEL = RATIO, INTERVAL, or LOGINTERVAL.
 - COEFF = IDENTITY | DIAGONAL, yields Euclidean distances and weighted Euclidean distances (“INDSCAL”), respectively.
- The Loss Function
 - FORMULA = 0 | 1 | 2 determines how the badness-of-fit criterion is standardized. 0 fits a regression model by ordinary least squares, not for level=ordinal. 1 is Stress-1 (for FIT = DISTANCE and LEVEL = ORDINAL) or S-Stress (for FIT = SQUARED and LEVEL = ORDINAL). 2 standardizes each partition specified by CONDITION; corresponds to Stress-2 for FIT = DISTANCE and LEVEL = ORDINAL. Default is 1 unless FIT = LOG.
 - ALTERNATE = NONE | MATRIX | ROW. Determines what form of alternating least-squares algorithm is used. NONE causes all parameters to be adjusted simultaneously on each iteration; best for small n (=objects) and N (=matrices). MATRIX adjusts the parameters for the first proximity matrix, then for the second, etc.; best for large N and small n . ROW adds further stages; best for large n .
 - FIT = DISTANCE | SQUARED | LOG | n specifies a fixed transformation to apply to *both* $f(p_{ij})$ s and d_{ij} s before the error is computed. This leads to different weighting of large/small values. The default is DISTANCE or, equivalently, 1 which fits $f(p_{ij})$ ’s to d_{ij} ’s. FIT = n fits n th power $f(p_{ij})$ s to n th power d_{ij} s.
 - Some technical options
 - MAXITER = k , the maximum number of iterations. Default is 100.
 - CONVERGENCE = k , the convergence criterion. Default is $k = .01$. Values of less than .0001 may be impossible because of machine precision.
 - RANDOM = k , causes initial coordinate values to be pseudorandom numbers with seed= k .
 - Some output options
 - PFIT and PCONFIG: print the fit values and the MDS configuration, respectively. Various other print options exists, e.g., PINIT, which prints the initial values, and PTRANS, which prints the estimated transformation parameters if any are computed in metric models.
 - OUT = xyz. Creates the SAS data file “xyz” containing the estimates of all parameters of the MDS model and the value of the badness-of-fit criterion.
 - OUTRES = xyz. Creates file that contains original proximities, MDS distances, transformed proximities/distances, residuals.

For more information, contact: SAS Institute Inc., 100 SAS Campus Drive, Cary, NC 27513-2414, U.S.A. Phone: (919) 677-8000. Fax: (919) 677-4444. Internet: <http://www.sas.com>

STATISTICA

STATISTICA is a comprehensive package for statistics and statistical graphics that includes an MDS module. Doing MDS, STATISTICA yields windows of numerical output, high-resolution plots of the MDS configuration (also 3D configurations that can be rotated in space), fit plots such as data vs. d-hats or data vs. rank-images, and so on. The graphics windows can be modified by changing fonts, changing the line thickness, resizing points, moving point labels as objects, and the like, or by drawing into the plots with the built-in drawing tools.

STATISTICA's MDS module uses the Guttman–Lingoes initial configuration or a user-supplied external initial configuration. It then employs the MINISSA algorithm (Roskam & Lingoes, 1981), which does ordinal MDS with rank-images in the initial iterations and monotone regression later on to ensure convergence. As fit indices, Stress and Raw Stress are computed with both monotone regression values and rank-images. The coefficient of alienation is also reported.

STATISTICA's MDS only offers ordinal MDS and the Euclidean metric. Although this is sufficient for most applications, models like interval MDS, say, are needed for some data to avoid degeneracies.

STATISTICA can be run interactively (via mouse clicks that can be recorded), by submitting a program of previously stored mouse clicks, or by executing a file of STATISTICA's SCL command language. In SCL, our politicians example is set up as shown below, assuming that a system file "proxpol.sta" has been created beforehand. There exists only one further option: ITERATIONS = k .

```
FILE = "c:\proxpol.sta"
MDS
  / VARIABLES = ALL
  / DIMENSIONS = 2
```

For more information, contact: StatSoft Inc., 2300 East 14th St., Tulsa, OK 74104, U.S.A. Phone: (918) 749-1119. Fax: (918) 749-2217. E-mail: info@statsoft.com. Internet: <http://www.statsoft.com>

SYSTAT

SYSTAT is a comprehensive package for statistics, including graphics (Wilkinson & Hill, 1994). SYSTAT can be run in batch mode, submit mode, interactive line mode, and in a pull-down menu mode. As is true for all statistics packages, it is best to first set up a system file containing the proximity matrix. System files are defined via a spreadsheet, reading data from an ASCII file, or by computing proximities internally from other data. However, data can also be input from within a command file. To do a SYSTAT MDS analysis, one calls, from within the MDS module, the system file "polit.syd", say,

by typing “USE polit” (return), followed by “MODEL var1..var5” (return) and “ESTIMATE” (return). Alternatively, one first defines a command file containing these three lines and then submits this command file. (The first three letters of the commands are sufficient.) This will do an ordinal MDS in 2D, using Euclidean distances. A more explicit batch mode command job is this:

```
BASIC
SAVE polit
TYPE=DISSIMILARITY
INPUT Humphrey McGovern Percy Wallace Nixon
DIAGONAL=ABSENT
RUN
1
5 2
7 10 9
6 8 4 3
~
MDS
USE polit
MODEL Humphrey..Nixon
ESTIMATE / LOSS=KRUSKAL, REG=MONOTONIC, DIM=2, R=2
```

If the batch job is called “mds.cmd”, it is run by typing “sysstat < mds.cmd” from the DOS prompt. The resulting configuration and its Shepard diagram are shown on the computer screen, where they can be fine-tuned, previewed, and sent to a printer. The results can also be saved, along with distances, d-hats, and residuals for further analyses. In combination with a built-in spreadsheet editor, the points in the configuration plot can be labeled. Using this feature, one can, for example, create a facet diagram, where the points are labeled by their codings on a particular facet (see Chapter 5). Three-dimensional plots with embedded axes, labels, surfaces, and the like, are also available.

For an experienced data analyst, SYSTAT is best used with its command language and submit files. All SYSTAT jobs can be documented and easily modified if needed. However, even using pull-down menus or Windows, command language files are automatically generated for previewing and saving.

A SYSTAT MDS job generally looks like this:

```
MDS
MODEL variables / options
CONFIG arguments
SAVE filename / arguments
ESTIMATE / options
```

- The MODEL options: ROWS = N and SHAPE = RECT | SQUARE: when doing unfolding, one needs to specify that the proximity matrix is “rectangular” with N rows; the number of columns corresponds to the number of objects n .

- The CONFIG arguments: CONFIG = [coordinates of first point; coordinates of second point; ...] or CONFIG = LAST. The LAST argument allows using the configuration from the previous scaling. An example for an external 3-point configuration in 2D is CONFIG = [1 2; 3.3 5; 4 5].
- The SAVE arguments: Specifying DISTANCES saves the MDS distances; CONFIG saves the final MDS configuration; RESID saves the proximities, distances, d-hats, and residuals, together with row and column subscripts.
- The ESTIMATE options:
 - DIMENSION = m specifies the dimensionality m of the MDS solution.
 - REGRESSION = MONOTONIC | LINEAR | LOG | POWER uses ordinal, interval, log-interval, or power-function MDS, respectively.
 - SPLIT = ROW is split-by-rows (unfolding); SPLIT = MATRIX is split-by-matrix conditionality for stacked proximity matrices.
 - WEIGHT is individual differences scaling with dimension weights for each matrix.
 - R = r specifies the exponent of the Minkowski metric. For example, R = 2 requests Euclidean distances.
 - LOSS = KRUSKAL | GUTTMAN | YOUNG specifies the loss function. KRUSKAL is Stress-1; GUTTMAN is the coefficient of alienation, K ; YOUNG is S-Stress.
 - ITERATIONS = k sets the maximum number of iterations to k .
 - CONVERGE = k causes MDS to stop when the maximum absolute difference between any coordinate in the solution \mathbf{X} at iteration i and iteration $i + 1$ is less than k .

The program defaults are DIM = 2, REGR = MONO, no split, no weight, LOSS = KRUS, R = 2, ITER = 50, DECREMENT = 0.005.

For more information, contact: Systat Software, Inc.; 501 Canal Blvd; Suite E; Point Richmond, CA 94804-2028; U.S.A. Phone: (800) 797-7401. Fax: (800) 797-7406. E-mail: info-usa@systat.com. Internet: <http://www.systat.com>

A.3 MDS Programs without High-Resolution Graphics

Most programs from the early days of MDS lack high-resolution graphics. Nevertheless, these programs are usually well documented in the literature and often used in simulation studies. For completeness, we discuss a few of these programs.

The Guttman–Lingoes Nonmetric PC Series

The GL Series is a collection of 32 individual programs for the analysis of qualitative and ordinal data. The philosophy of the GL Series is to have compact programs that are good for particular purposes rather

than one jumbo program that does everything. For MDS, the main program is MINISSA-I for unconditional and row/column conditional proximities, but there are also special programs for proximities that are both row and column conditional at the same time (SSA-II), for imposing a number of independent sets of order constraints onto the distances (CMDA), for individual differences scaling (PINDIS), or for representing proximities in a vector model (SSA-III). A complete documentation of the source code (FORTRAN IV) of most of the programs is available (Lingoes, 1973).

The GL programs are essentially batch programs. The user is required to “punch” his or her specifications as numbers in four-field columns of the parameter “cards” of the batch job (see below, fourth row of batch job). A typical set-up for MINISSA-I for our politicians data looks as follows.

```
SSA-I.OUT (name of file for numerical output)
SSA-I.PLT (name of file for printer-plot output)
1 MDS of five politicians ("title card")
  5  2  2  0  0  1  0  0  0  0  0  0  0  0  0
(5F3.0)
  1
  5  2
  7 10  9
  6  8  4  3
```

The various numerical entries on the fourth “card” specify the number of objects (5), the lowest MDS dimensionality (2), the highest MDS dimensionality (2), the type of proximities (0=dissimilarities), a request to print out the distance matrix (0=no), and a request to minimize Kruskal’s Stress (1=yes). The remaining zeros refer to the usual defaults: Adding points to a fixed configuration (no=0, yes=1), external initial configuration (no=0, yes=1), special switch for program options (0=no special setting, 1=ignore cells in SSA-I/MDS, number of column fields for SSAR-I/unfolding), ignore cells in data matrix (no=0, yes=1), missing data (no=0, yes=1), distance formula (Euclidean=0, city-block=1), differential weighting of small and large distances (global weighting=0, local weighting=1), type of analysis (SSA-I/MDS=0, SSAR-I/unfolding=1), missing data code (real value), value above/below which all input data are considered tied (real value).

Most of the GL programs can be downloaded from <http://www.newmdsx.com>

FSSA: *Faceted Smallest Space Analysis*

A special MDS program is FSSA by Shye (1991). FSSA is a stand-alone program that is public domain for scientists. It analyzes from 3 to 50 objects in two to ten dimensions, using the Guttman algorithm. What makes FSSA unique is that it allows one to code the objects with respect to several facets (see Chapter 5). FSSA then partitions the resulting 2D planes, facet by facet, in three ways (axial, polar, modular), using parallel straight lines, concentric circles, and rays emanating from a common origin, respectively. The partitionings are shown as screen diagrams.

The program can be obtained from: Samuel Shye, Dept. of Psychology, Hebrew University of Jerusalem, Jerusalem 91905, Israel. E-mail: msshye@pluto.mscc.huji.ac.il

KYST

KYST (Kruskal et al., 1978) is an exceedingly flexible MDS program. It allows one to set up virtually any MDS model, except MDS with side constraints on coordinates or distances. KYST is noncommercial software, available on the Internet at <http://www.netlib.org/mds/>. The program is written in FORTRAN and can, in principle, be compiled on any machine. KYST allows the user to specify Minkowski distances other than the Euclidean distance. Moreover, weights can be assigned to each proximity, for example, for weighting each datum by its reliability. Another feature is the possibility of polynomial regression for specifying the transformation function of the proximities. Because KYST is an old program, it provides only printer-type graphics with 132 characters per line. KYST's manual is not made for today's occasional user of MDS, but the logic of KYST's command language is straightforward.

An example setup for a KYST2e job is the following.

```
DIMMAX = 2, DIMMIN = 2
REGRESSION = ASCENDING
COORDINATES = ROTATE
ITERATIONS = 100
PRINT = HISTORY
PRINT = DATA
PLOT = SCATTER = ALL
PLOT = CONFIGURATION
TORSKA
DATA, LOWERHALFMATRIX, DIAGON = ABSENT
KYST example setup: politicians
  5  1  1
(5F3.0)
  1
  5  2
  7 10  9
  6  8  4  3
COMPUTE
STOP
```

The setup consists of control lines and the data definition lines (data deck). The order of the control lines mostly does not matter. The data definition lines start in this example with the line "DATA, LOWERHALFMATRIX,..." and end with the line "6 8 4 3". These lines are in strict order and may not be reordered. Also, the REGRESSION control lines should precede the data definition lines. Some of the control commands on the control lines are:

- Analysis options: DIMMAX = 3 sets the maximum dimensionality to 3, DIMMIN = 2 sets the minimum dimensionality to 2. SFORM1 makes the program use Kruskal's Stress formula 1, SFORM2 requests Kruskal's Stress formula 2. PRIMARY requests

the primary approach to ties, and SECONDARY the secondary approach. ITERATIONS = 100 sets the maximum number of iterations to 100, SRATST = 0.9999 causes KYST to stop the iterations whenever the ratio of subsequent Stress values is smaller than 0.9999. STRMIN = .00001 stops the iterations if the Stress becomes smaller than .00001. TORSKA takes the classical scaling solution as the initial configuration. COORDINATES = ROTATION causes the solution to be rotated to principal axes (recommended).

- REGRESSION specifies the type of admissible transformation of the proximities. REGRESSION = ASCENDING indicates that the proximities are dissimilarities, REGRESSION = DESCENDING that they are similarities. REGRESSION = POLYNOMIAL = 3 specifies a third-degree polynomial regression transformation. Adding REGRESSION = CONSTANT (or NOCONSTANT) makes the program pick an optimal additive constant. Thus, an interval transformation is specified by REGRESSION = POLYNOMIAL = 1, REGRESSION = CONSTANT.
- Print and plot options. PRINT = (NO)DATA prints the proximities, PRINT = (NO)HISTORY outputs the history of iterations, and PRINT = (NO)DISTANCES prints the distances and the disparities. When a range of dimensions is specified, a plot of Stress against the number of dimensions is given. PLOT = SCATTER = ALL (or = NONE for no plots) produces a plot of distances and disparities against the proximities. PLOT = CONFIGURATION = ALL (or =SOME or = NONE) causes KYST to plot all principal components projection planes of the MDS configuration. SOME only plots the first principal component against all other components.
- Data definition. The data are defined by five parts: (1) a line ("card") specifying the data; (2) a title line; (3) a line of parameters; (4) a line with the format of the data; (5) lines specifying the data. Line 1 of the data definition part starts with DATA followed by LOWERHALFMATRIX to indicate the lower triangular elements, UPPERHALFMATRIX indicates the upper triangular elements, and MATRIX specifies the full matrix. For triangular matrices, one specifies either DIAGONAL = PRESENT or = ABSENT. For unfolding, one sets LOWERCORNERMATRIX (or UPPERCORNERMATRIX). Line 3 expects 3 or 4 numbers that should end in columns 3, 6, 9, and 12, respectively. The parameters specify number of objects, number of replications (usually 1), number of groups (usually 1), respectively. For corner matrices, the parameters are: number of rows; number of columns; the number of replications; number of groups. Line 4 contains a FORTRAN format, for example, (5F10.3). Line 5 (and further) contains the data, possibly followed by weights. The weights definition block is specified in the same way as the data definition block, except that the word DATA has to be replaced by WEIGHTS.
- COMPUTE causes the program to start computing. After the COMPUTE command, further MDS jobs can be set up, before a final STOP.

For more information contact: Scott M. Smith, Ph.D., Dept. of Marketing, 634 TNRB Brigham Young University, Provo, Utah 84602, U.S.A. E-mail: smsmith@byu.edu. Phone: (801) 376-1339. Fax: (801) 705-9430. Internet: <http://marketing.byu.edu>

MULTISCALE

MULTISCALE (Ramsay, 1977) is one of the few MDS programs that offers a Maximum Likelihood (ML) approach. For ML, it can assume normal

or lognormal distributions of the residuals and assumes that the errors are independent. MULTISCALE is one of the few programs that yields confidence regions for each point. The program has various options, including, for example, spline transformations, power transformations, and the weighted Euclidean model. The output of this program is somewhat hard to read because it contains much statistical information. However, the program has a clearly written manual. The MS-DOS version of MULTISCALE has high-resolution graphics and can output postscript plots. MULTISCALE runs on several operating systems.

A sample setup for MULTISCALE is

```
@TITLE LINES=2;
  Example setup of {\sc Multiscale}:
  similarity of 5 politicians,
@PARAMETERS NSTIM=5, NSUB=1, NDIM=2,
              TRAN=SPLINES, DISTRIB=LOG;
@DISDATA VECTOR FORMAT=FREE;
1
5 2
7 10 9
6 8 4 3
@STIMLABS FORMAT=FREE;
Humphrey McGovern Percy Wallace Nixon
@COMPUTE;
```

MULTISCALE has its own command language. The following summarizes the most important commands. The input of MULTISCALE is organized in blocks. Each block starts with an @ and ends with a semicolon (;). For example, there exists a block for the title, a block for the parameters of the analysis, and a block for reading the data. For the most part, these blocks can appear in any order, with the following exceptions: the PARAMETER block must be the first block or the second block just after the TITLE block, and the COMPUTE block is the last block before the analysis takes place. Several runs can be specified in one file by repeating a (possibly different) PARAMETER (and TITLE) block ended by the next COMPUTE block.

Here is a short description of some of the blocks:

- The TITLE block indicates that the next line is a title. LINES = 2 specifies that the title has two lines (maximum is five lines).
- The PARAMETER block sets all the important options of the analysis. NSTIMULI defines the number of objects, NDIMENSIONS sets the number of dimensions, NSUBJECTS specifies the number of replications, NKNOTS sets the number of interior knots when using spline transformation, PROBABILITY sets the confidence level for the confidence regions for points, METRIC = IDENTITY (default) for weighting every dimension equal and METRIC = DIAGONAL for weighting each dimension separate (needed for the weighted Euclidean model). TRANSFORM sets the transformation of the proximities: the keyword SCALE sets the disparity (optimally) to the sum of the proximity and an additive constant only, POWER assumes interval level of the proximities, SPLINE specifies monotone splines. With DISTRIBUTION = LOGNORMAL, we assume that the error distribution is lognormal (default); with NORMAL, we simply obtain the Stress function. DCOMPLETE indicates that the complete proximity matrix is available for each replication instead of the lower triangular elements, LISTDATA prints input matrices, NOSTATS avoids printing statistics

for replications, NOASYMPT avoids printing asymptotic variance estimates, NODIST suppresses the matrix of distances, and TABLES prints the matrix of disparities, distances and normalized residuals for each replication. DPLOT plots the disparities against the distances, TPLOT plots the disparities against the proximities, and QPLOT plots the normalized residuals against quantiles of the normal distribution. For preference data, specify PCOMPLETE for complete preference matrix instead of lower triangular elements, PLOT for plotting the preference against predicted preference.

- The DISDATA block inputs the proximities. MULTISCALE assumes that the proximities are entered in lower triangular format. However, VECTOR indicates that the proximities are in one large vector, not in lower triangular format. DIAGONAL specifies that diagonal values are present. FORMAT = fixed specifies that the data are read by a FORTRAN format, which is entered before the first line of data. FORMAT = FREE lets MULTISCALE read the data in free format, which means that the proximities should be separated by a space or a comma.
- The STIMLABELS block allows you to input labels of the objects. The labels should be on the lines following this block. By specifying FORMAT=FREE, the labels have to be separated by a space or a comma. In the same way, the SUBLABELS block allows you to specify labels for the replications.
- The COMPUTE block starts the analysis. ITMAX=100 sets the maximum number of iterations to 100, and CONV=.005 sets a convergence criterion dependent on the log-likelihood.

The program can be obtained free of charge from: James O. Ramsay, Dept. of Psychology, McGill University, 1205 Docteur Penfield Avenue, Montreal, Québec H4A 1B1, Canada. E-mail: ramsay@psych.mcgill.ca, Internet: <ftp://ego.psych.mcgill.ca/pub/ramsay/multiscl/>

Appendix B

Notation

For convenience, we summarize the notation used throughout this book. We use the following conventions: a lowercase italic character denotes a scalar, a lowercase bold character denotes a vector, and an uppercase bold character denotes a matrix. Elements of vectors or matrices are denoted by a subscripted scalar. A function is usually denoted by a character followed by an argument in parentheses, for example, $f(\mathbf{x})$ is a scalar function of the vector \mathbf{x} , and $\mathbf{A}(\mathbf{x})$ is a matrix function of the vector \mathbf{x} . Some explicit notation follows below.

n	Number of objects, persons, and so on.
i, j	Running index for objects, $i, j = 1, \dots, n$.
m	Number of dimensions.
a	Running index for dimensions, $a = 1, \dots, m$.
\mathbf{X}	Matrix of coordinates x_{ia} of n objects on m dimensions.
p_{ij}	Proximity between object i and j . It could be either a similarity or a dissimilarity measure.
δ_{ij}	Nonnegative dissimilarity between object i and j .
Δ	Symmetric matrix of nonnegative dissimilarities δ_{ij} of size $n \times n$, with $\delta_{ii} = 0$.

- $d_{ij}(\mathbf{X})$ The Euclidean distance between row i and row j of \mathbf{X} ; that is, $d_{ij}^2(\mathbf{X}) = \sum_{a=1}^m (x_{ia} - x_{ja})^2$.
- d_{ij} A shorter notation for the Euclidean distance $d_{ij}(\mathbf{X})$.
- \hat{d}_{ij} Disparity between objects i and j . Disparities are admissibly transformed proximities that optimally approximate given distances.
- w_{ij} A nonnegative weight used to (down)weight the residual in the Stress function.
- \mathbf{W} Symmetric matrix of weights w_{ij} with zero diagonal.
- $\mathbf{D}(\mathbf{X})$ Matrix of Euclidean distances between the rows of \mathbf{X} .
- \mathbf{A}' The transpose of \mathbf{A} .
- \mathbf{I} The identity matrix, which is a square matrix with diagonal elements equal to 1 and off-diagonal elements equal to 0.
- $\mathbf{1}$ A column vector with all elements equal to 1.
- \mathbf{J} The $n \times n$ centering matrix, $\mathbf{J} = \mathbf{I} - n^{-1}\mathbf{1}\mathbf{1}'$, where all elements of the matrix $\mathbf{1}\mathbf{1}'$ are equal to 1.
- \mathbf{A}^q The q th power of a square matrix \mathbf{A} . For example, $\mathbf{A}^3 = \mathbf{A}\mathbf{A}\mathbf{A}$.
- \mathbf{A}^{-1} The matrix inverse of a square matrix \mathbf{A} assuming that \mathbf{A} is of full rank, so that $\mathbf{A}^{-1}\mathbf{A} = \mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$.
- \mathbf{A}^{-} A generalized inverse of a square matrix \mathbf{A} where \mathbf{A} may be rank deficient, so that $\mathbf{A}\mathbf{A}^{-}\mathbf{A} = \mathbf{A}$ and $\mathbf{A}^{-}\mathbf{A}\mathbf{A}^{-} = \mathbf{A}^{-}$ holds. Usually, we choose the Moore–Penrose inverse \mathbf{A}^{+} as the generalized inverse.
- $\mathbf{A}^{(2)}$ Matrix \mathbf{A} with squared elements.
- $\mathbf{A}(\mathbf{X})$ Any matrix function of \mathbf{X} with elements $a_{ij}(\mathbf{X})$.
- $\text{tr } \mathbf{A}$ The trace operator sums the diagonal elements of \mathbf{A} ; that is, $\text{tr } \mathbf{A} = \sum_{i=1}^n a_{ii}$.
- $\hat{\phi}(\mathbf{x}, \mathbf{y})$ Majorizing function of $\phi(\mathbf{x})$ for which $\phi(\mathbf{x}) \leq \hat{\phi}(\mathbf{x}, \mathbf{y})$ and $\phi(\mathbf{x}) = \hat{\phi}(\mathbf{x}, \mathbf{x})$ holds for all feasible \mathbf{x} and \mathbf{y} .
- $\|\mathbf{X}\|$ The Euclidean norm of matrix \mathbf{X} ; that is, $\|\mathbf{X}\|^2 = \sum_{i=1}^n \sum_{a=1}^m x_{ia}^2$.
- $\|\mathbf{X}\|_{\mathbf{V}}$ The weighted Euclidean norm of matrix \mathbf{X} ; that is, $\|\mathbf{X}\|_{\mathbf{V}}^2 = \text{tr } \mathbf{X}'\mathbf{V}\mathbf{X}$.

σ_r	Raw Stress, that is, the sum of the squared differences between the optimally transformed proximities $f(p_{ij})$ (i.e., the disparities \hat{d}_{ij}) and the corresponding distances $d_{ij}(\mathbf{X})$ of the MDS configuration \mathbf{X} .
σ_n	Normalized Stress, that is, raw Stress divided by the sum of squared dissimilarities or disparities.
σ_1	Stress formula 1, that is, the square root of raw Stress divided by the sum of squared distances.
σ_2	Stress formula 2, that is, the square root of raw Stress divided by the sum of squares of the distances minus the average distance.

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