Statistics for the Sciences

Multidimensional Scaling

Xuemao Zhang East Stroudsburg University

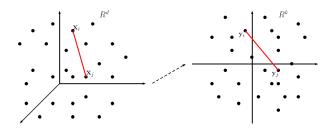
January 18, 2025

Outline

- Purpose of multidimensional scaling
- Multidimensional Scaling (MDS)
 - metric MDS
 - non-metric MDS
- Example
- Lab

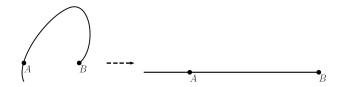
Purpose of multidimensional scaling

- Multidimensional scaling (MDS) is another technique on dimensionality reduction.
- Unlike PCA, MDS maps the original high dimensional space to a lower dimensional space, but does so in an attempt to preserve pairwise distances.
 - ▶ The space is usually two-dimensional, sometimes may be three-dimensional.



Purpose of multidimensional scaling

- The purpose of MDS is often just visualizing the data so it becomes easier for the user to explore and to understand their structure.
- The MDS algorithm starts with a distance matrix and uses it to reduce the data to two dimensions while preserving the pairwise distances.
 - PCA starts with the correlation matrix of data.



- MDS methods include
 - Classical MDS (Metric MDS) or Principal Coordinates Analysis (PCoA),
 - Non-metric MDS which focuses on preserving the rank order of the dissimilarities rather than the actual distances.

• Given p-dimensional data, how do we construct a **distance** matrix?

$$\mathbf{X} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix}$$

- Distance, dissimilarity and similarity (or proximity) are defined for any pair
 of objects in any space.
 - ▶ Each objects or subject is just a row (record) of observations.
- Let x, y, z be objects. In mathematics, a distance function (that gives a distance between two objects) is also called metric. satisfying
 - $d(x, y) \geq 0$
 - d(x,y) = 0 if and only if x = y
 - d(x,y) = d(y,x)
 - \rightarrow $d(x,z) \leq d(x,y) + d(y,z)$
- Given a set of dissimilarities, one can ask whether these values are distances.

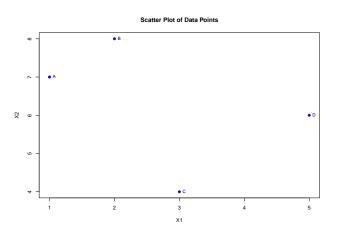
- Dissimilarity Matrix: $n \times n$ with the ij-th element d_{ij} measuring the distance (similarity or proximity) between the ith and the jth objects (or observations). D is symmetric.
 - ▶ Here *p* is the dimension of the data or the number of variables.
- Dissimilarity between points i and i': \mathbf{x}_i and $\mathbf{x}_{i'}$ (i, i' = 1, ..., n):

$$d(\mathbf{x}_i,\mathbf{x}_{i'}) = \sum_{j=1}^p d_j(x_{ij},x_{i'j}).$$

An example

```
## x1 x2
## A 1 7
## B 2 8
## C 3 4
```

• A scatter plot of these data



Construct a dissimilarity matrix

```
## [1] "Distance matrix of the data:"

## A B C D

## A 0.000000 1.414214 3.605551 4.123106

## B 1.414214 0.000000 4.123106 3.605551

## C 3.605551 4.123106 0.000000 2.828427

## D 4.123106 3.605551 2.828427 0.000000
```

- There are several types of distances. Consider two points $A(x_1, y_1)$ and $B(x_2, y_2)$
 - Euclidean distance $d(A, B) = \sqrt{(x_1 x_2)^2 + (y_1 y_2)^2}$
 - ► Maximum Distance $d(A, B) = max(|x_1 x_2|, |y_1 y_2|)$
 - ► Manhattan Distance $d(A, B) = |x_1 x_2| + |y_1 y_2|$
 - ▶ Bray Distance $d(A, B) = \frac{|x_1 x_2|}{|x_1| + |x_2|} + \frac{|y_1 y_2|}{|y_1| + |y_2|}$
 - Minkowski Distance $d(A, B) = [(x_1 x_2)^p + (y_1 y_2)^p]^{1/p}, p > 0$
 - ▶ Binary Distance (Dissimilarity for binary data) $d(A, B) = (x_1 \text{ XOR } x_2) + (y_1 \text{ XOR } y_2)$

The MDS problem:

- Assume a collection of *p*-dimensional *n* objects with Dissimilarity Matrix $\mathbf{L} = \{l_{ii}\}, i, j = 1, 2, ..., n.$
- Our objective is to represent them as points in 2-d Euclidean space, $\mathbf{y}_1, \dots, \mathbf{y}_n \in \mathbb{R}^2$, such that

$$d_{ij} = d_{\mathbf{y}_i,\mathbf{y}_i} = I_{ij}$$
 or as close as possible for any i,j .

- MDS
 - ► Called **metric MDS** if dissimilarities *l_{ii}* are quantitative.
 - ▶ Called **non-metric MDS** if dissimilarities l_{ij} are qualitative (e.g. ordinal).

- The mathematical tool for MDS often involves eigen decomposition of the Dissimilarity matrix to transform the distance information into a lower-dimensional space while preserving the distances between data points.
- Solution to MDS is not unique.
 - ▶ If **Y** is a solution, then $\mathbf{Y}^* = \mathbf{Y} + \mathbf{c}, \mathbf{c} \in \mathbb{R}^2$ is also a solution.
 - **c** is just a location transformation.

Non-metric MDS

- In many applications of MDS, dissimilarities are known only by their rank order, and the spacing between successively ranked dissimilarities is of no interest or is unavailable.
 - ▶ Non-metric MDS focuses on preserving the rank order of the dissimilarities.
- \bullet Non-metric MDS: non-metric MDS seeks to find an optimal configuration $\textbf{Y} \subset \mathbb{R}^2$ such that

$$f(I_{ij}) \approx d_{\mathbf{y}_i,\mathbf{y}_j} = d_{ij}$$
 for any i,j .

where f is a general monotonic function implicitly defined by the rank order of the original dissimilarities l_{ij} .

• $f(l_{ij})$ generates **disparities**, which only preserve the order of the original dissimilarities l_{ii} . That is

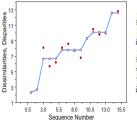
$$I_{ij} < I_{i'j'} \Leftrightarrow f(I_{ij}) < f(I_{i'j'})$$

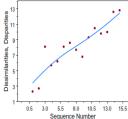
Non-metric MDS

Kruskal's non-metric MDS minimizes the stress-1

$$\mathsf{stress-1}(f(\mathit{l}_{ij}), \mathit{d}_{ij}) = \left(\sum_{i < j} \frac{(f(\mathit{l}_{ij}) - \mathit{d}_{ij})^2}{\sum \mathit{d}_{ij}^2}\right)^{1/2}$$

- It quantifies the difference between the disparities $f(I_{ij})$ and the distances d_{ii} in \mathbb{R}^2 .
- The function f works as if it were a regression curve
 - ightharpoonup approximated dissimilarities d_{ij} treated as response,
 - \blacktriangleright disparities $f(I_{ij})$ serves as estimate average of the response, and
 - ▶ the order of dissimilarities as explanatory
 - ▶ In the following figure, Left panel: Isotonic regression. right panel: Monotone spline. For the red points, the vertical axis is the dissimilarity I_{ij} , whereas for the fitted blue points, the vertical axis is the disparity $f(I_{ii})$.





Xuemao Zhang East Stroudsburg University

Statistics for the Sciences

January 18, 2025

Non-metric MDS

Process of Non-metric MDS

- ▶ Initialization: Start with an initial configuration of points in the lower-dimensional space like \mathbb{R}^2 .
- Compute Distances: Calculate the Euclidean distances d_{ij} between points in the current configuration.
- ▶ Monotonic Regression: Find the disparities $f(l_{ij})$ that best match the distances d_{ij} while preserving the rank order of l_{ij} .
- ▶ Optimization: Adjust the configuration of points (the coordinates of y) to minimize the stress function in the last slide. The goal is to find the configuration where the distances d_{ij} are as close as possible to the disparities $f(l_{ij})$.

- lemminvert.csv: Lemmens et al. (2015) did a detailed study of various biotic communities in artificial ponds in Belgium. They sampled 28 ponds that represented different types of management, a combination of fish farming strategies (no fish, farming young fish, low intensity management, no management), and drainage frequencies (> 10 years ago, occasional, annual). They also quantified taxon abundances for fish, zooplankton, and macro-invertebrates (different families and species within some groups) and covers of submerged, floating, and emergent vegetation. The macroinvertebrate dataset only included 23 ponds.
- See analysis with R here: https://mjkeough.github.io/examples/lemmpcoa.nb.html

```
## [1] "1J1" "1J2" "1J3" "1J5" "1J6" "1J7" "BK1" "BK2" "BK5" "BK6" ## [13] "02" "03" "04" "05" "06" "07" "V1" "V2" "V3" "V4"
```

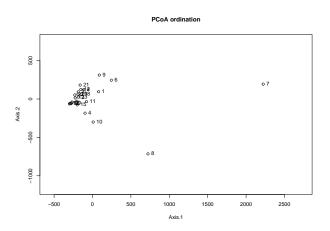
• The first 3 variables are pond classification variables

```
23 obs. of 32 variables:
## 'data frame':
              : Factor w/ 23 levels "1J1", "1J2", "1J3", ...: 1 2 3 4 5 6 7 8 9 10 ....
##
   $ site
##
   $ manag
              : Factor w/ 4 levels "li", "nf", "nm", ...: 4 4 4 4 4 4 2 2 2 2 ...
   $ managsymb: int
                   0 0 0 0 0 0 1 1 1 1 ...
   $ caen
              : int
                    0 6 0 5 0 3 31 36 0 16 ...
##
   $ baet
              : int 158 13 20 98 3 605 1571 494 73 90 ...
   $ acrol
                   0 0 0 0 0 0 0 0 1 0 ...
##
              : int
##
   $ lvmn
              : int
                   3 0 3 10 9 7 763 109 46 15 ...
   $ plan
                   5 50 16 206 14 19 1164 1035 64 421 ...
##
              : int
##
   $ sphaer
              : int
                   0 0 0 2 0 0 80 147 0 0 ...
##
   $ vivip
              : int
                   0000000000...
   $ corix
              : int
                   671 95 8 98 23 9 730 389 239 25 ...
##
##
   $ nauc
              : int
                   0 0 0 0 0 0 0 2 2 0 ...
   $ nepid
##
              : int 0000000000...
##
   $ noto
              : int
                    0 0 0 0 0 0 3 1 0 0 ...
##
   $ pleid
              : int
                    0 0 0 0 0 0 20 141 5 0 ...
   $ gamm
##
              : int.
                   0 0 1 2 1 0 4 0 4 1 ...
##
   $ asell
              : int
                   0 0 0 4 0 0 0 0 0 1 ...
##
   $ cerat
                   4 7 9 5 0 7 88 3 6 20 ...
              : int
   $ chaob
                   23 37 60 20 3 5 68 0 204 22 ...
              : int
##
   $ chiro
              : int
                   222 322 240 26 60 394 1236 62 569 69 ...
   $ culic
##
              : int 19 17 12 4 3 19 12 0 24 21 ...
##
   $ cylind
                   00000000000...
              : int
##
   $ dixid
              : int
                    40 52 30 2 5 0 4 6 47 38 ...
   $ empid
##
              : int
                    0 0 0 0 1 0 0 0 0 5 ...
##
   $ ephyd
              : int
                    0 0 0 0 1 0 0 0 0 0 ...
##
   $ limon
                     8 1 25 9 2 0 8 0 0 10 ...
              : int
```

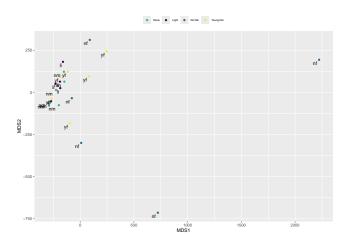
PCoA Analysis

```
## $correction
## [1] "none" "1"
##
## $note
## [1] "There were no negative eigenvalues. No correction was applied"
## $values
       Eigenvalues Relative eig Broken stick Cumul eig Cumul br stick
## 1 6.284770e+06 7.820467e-01 0.167764239 0.7820467
                                                            0.1677642
     9.438104e+05 1.174433e-01
                                0.122309693 0.8994900
                                                            0.2900739
     4.249575e+05 5.287968e-02
                                 0.099582420 0.9523696
                                                            0.3896564
## 4 2.622459e+05 3.263263e-02
                                 0.084430905 0.9850023
                                                            0.4740873
## 5 7.088309e+04 8.820352e-03
                                0.073067269 0.9938226
                                                            0.5471545
## 6 2.045955e+04 2.545889e-03 0.063976360 0.9963685
                                                            0.6111309
## 7 1.124622e+04 1.399426e-03
                                0.056400602 0.9977679
                                                            0.6675315
## 8 5.798579e+03 7.215475e-04
                                0.049907096 0.9984895
                                                            0.7174386
## 9 5.194204e+03 6.463420e-04
                                0.044225278 0.9991358
                                                            0.7616639
## 10 2.820873e+03 3.510159e-04
                                 0.039174773 0.9994868
                                                            0.8008386
## 11 1.844753e+03 2.295523e-04
                                0.034629318 0.9997164
                                                            0.8354680
## 12 1.287003e+03 1.601485e-04
                                0.030497087 0.9998765
                                                            0.8659650
## 13 5.023922e+02 6.251528e-05
                                0.026709208 0.9999391
                                                            0.8926742
## 14 2.379086e+02 2.960421e-05
                                0.023212704 0.9999687
                                                            0.9158870
## 15 1.646356e+02 2.048647e-05
                                 0.019965951 0.9999891
                                                            0.9358529
## 16 4.038504e+01 5.025321e-06
                                0.016935648 0.9999942
                                                            0.9527886
## 17 2.848683e+01 3.544765e-06
                                0.014094739 0.9999977
                                                            0.9668833
## 18 8.453043e+00 1.051856e-06
                                0.011420942 0.9999988
                                                            0.9783042
## 19 4.215181e+00 5.245170e-07
                                0.008895690 0.9999993
                                                            0.9871999
## 20 3.346910e+00 4.164734e-07
                                 0.006503345 0.9999997
                                                            0.9937033
                                                            0.9979339
## 21 1.664062e+00 2.070680e-07
                                 0.004230618 0.9999999
## 22 6.604191e-01 8.217940e-08
                                0.002066116 1.0000000
                                                            1.0000000
##
## $vectors
           Axis.1
                     Axis.2
                                 Axis.3
                                             Axis.4
                                                         Axis.5
                                                                      Axis.6
       79.740869
                   95.10472 498.99343
                                        215.307907 -38.041790 -21.18016513
     -114 437233
                 122.79086
                               36.06851 -115.990258
                                                    -23 898179 -39 23757341
## 3 -185,375472
                   92.69808 -47.57754 -84.558400 -12.730992
                                                                  2.97584395
## 4 -96.499521 -184.16382 -11.40450 17.971440
                                                      8.590388 -0.03897887
Xuemao Zhang East Stroudsburg University
                                                     Statistics for the Sciences
```

biplot



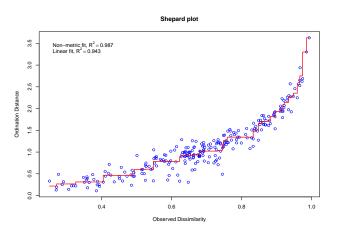
biplot



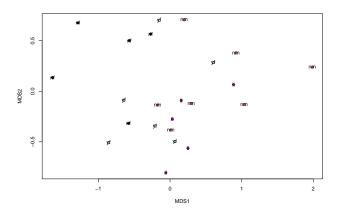
 NDMS using bray distance https://mjkeough.github.io/examples/lemmmds.nb.html

```
## Run 0 stress 0.1156702
## Run 1 stress 0.1153229
## ... New best solution
## ... Procrustes: rmse 0.01893663 max resid 0.07573146
## Run 2 stress 0.115323
## ... Procrustes: rmse 0.0002871722 max resid 0.001111882
## ... Similar to previous best
## Run 3 stress 0.1153229
## ... New best solution
## ... Procrustes: rmse 0.0001334567 max resid 0.0005117371
## ... Similar to previous best
## Run 4 stress 0.115323
## ... Procrustes: rmse 0.0002058442 max resid 0.0008060438
## ... Similar to previous best
## Run 5 stress 0.1153229
## ... Procrustes: rmse 0.0001425949 max resid 0.0005563484
## ... Similar to previous best
## Run 6 stress 0.1172332
## Run 7 stress 0.1156703
## ... Procrustes: rmse 0.01890827 max resid 0.07510586
## Run 8 stress 0.11567
## ... Procrustes: rmse 0.01893865 max resid 0.07545109
## Run 9 stress 0.1156703
## ... Procrustes: rmse 0.0189112 max resid 0.07523154
## Run 10 stress 0.1172331
## Run 11 stress 0.1156701
```

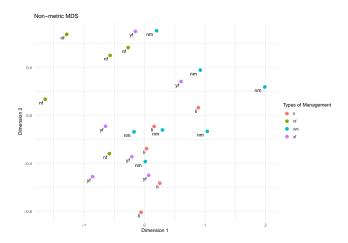
Stress plot



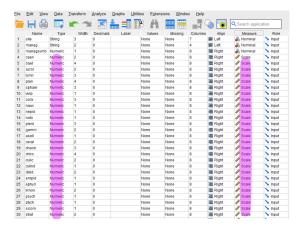
biplot



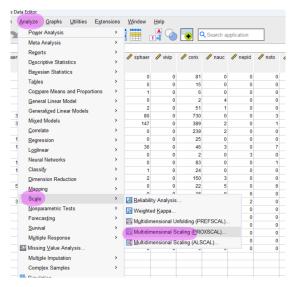
biplot



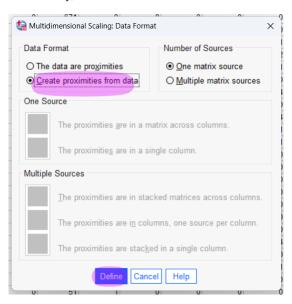
After importing data, change the measures of all numercal variables to Scale



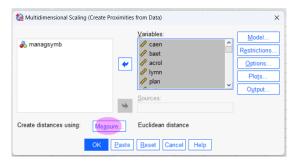
- ullet Go to Analyze o Scale o Multidimensional Scaling (ProxSCAL)....
 - ► PROXSCAL is for metric and non-metric MDS



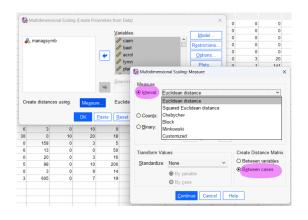
• We have raw data only, so we need to construct a distance matrix



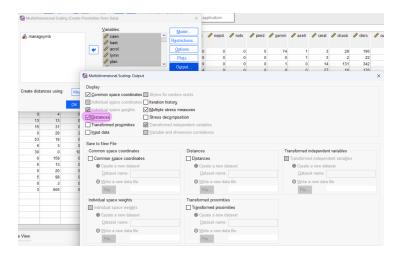
• Move all numerical variables to the Variables box



- Suppose we use Euclidean distance
 - ▶ Make sure we create distance matrix **Between cases**



Output options



- Stress Value: This measures the goodness-of-fit of the MDS solution. Lower values indicate a better fit.
 - ► Typically, stress values below 0.1 indicate a good fit.

Stress and Fit Measures

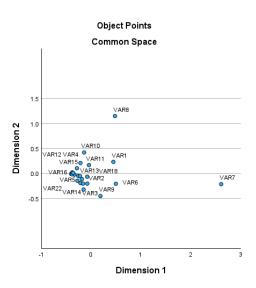
Normalized Raw Stress	.00753
Stress-I	.08678*
Stress-II	.11662ª
S-Stress	.01063 ^b
Dispersion Accounted For (D.A.F.)	.99247
Tucker's Coefficient of Congruence	.99623
DROVECAI minimina Manna	lined Dam

PROXSCAL minimizes Normalized Raw Stress.

- a. Optimal scaling factor = 1.003.
- b. Optimal scaling factor = .994.

Final Coordinates

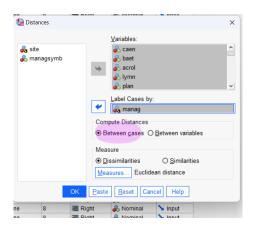
	Dimension								
-	1	2							
VAR1 Case 1	.445	.231							
VAR2 Case 2	079	206							
VAR3 Case 3	215	194							
VAR4 Case 4	216	.208							
VAR5 Case 5	338	025							
VAR6 Case 6	.494	209							
VAR7 Case 7	2.610	218							
VARS Case S	.478	1.148							
VAR9 Case 9	.185	455							
VAR10 Case 10	142	.418							
VAR11 Case 11	046	.166							
VAR12 Case 12	404	010							
VAR13 Case 13	- 261	051							
VAR14 Case 14	- 166	205							
VAR15 Case 15	287	.102							
VAR16 Case 16	382	.020							
VAR17 Case 17	- 386	019							
VAR18 Case 18	081	067							
VAR19 Case 19	- 188	115							
VAR20 Case 20	362	.008							
VAR21 Case 21	154	325							
VAR22 Case 22	279	148							
VAR23 Case 23	- 226	055							



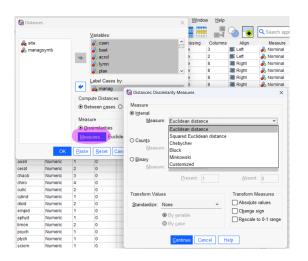
Distance matrix

Distances																							
	VARI Cust I	VAR2 Care 2	VARI Case I	VARICION 4	TARS Day 5	VARS Case 6	VAR7 Class 7	TARE CHASE	VARF Case F	VARIO Cus III	VARII Care II	VARIT Care 12	VARII Case 11	VARIACION 14	VARISCHI IS	VARIS Chier 16	VARIT Chir IT	VARIE Cur II	VARIF Care IF	VARIO Care 20	VARNI Case 21	VAR22 Case 22	VARITORS II
VARI Cust 1	.000																						
VAR2 Case 2	.682	.000																					
VAR3 Cere 3	.766	.137	000																				
VARACion 4	.663	.435	402	.000																			
VARS Cese 5	834	31.6	210	.263	.000																		
VAIM Cent 6	.442	.573	710	324	533	800																	
VAR7 Case 7	2.211	2.689	2.836	2.858	2.955	2.116	.000																
VAR3 Cere 3	.913	1.464	1.50	1.169	1.429	1.338	2.532	.000															
VARS Cape 9	.733	363	472	.775	672	295	2.436	1.630	200														
VARIO Cere 10	.617	627	617	.223	.484	294	2.825	938	932	.000													
VARII Cure 11	405	373	375	.176	340	457	2.693	1.113	552	270	.000												
VARI2 Care 12	223	300	354	.293	D63	920	3.022	1.456	130	.502	400	000											
VAB13 Cere 13	.760	239	151	.262	.002	.771	2.876	1.408	802	464	305	149	900										
VARI4 Care 14	.724	007	0.51	404	249	550	2.776	1.499	431	.634	370	300	191	000									
VARIS Care 15	744	371	305	.127	137	34)	2915	1.296	.730	348	150	362	155	330	.000								
VARIA Curv 16	.033	377	271	.230	.062	905	3.001	1.413	340	465	366	130	140	312	125	.000							
VARI7 Care 17	263	339	345	.293	D42	901	3.003	1.452	719	.501	327	830	139	200	1.56	039	000						
VARIS Cere 15	605	138	185	307	.261	.992	2.695	1.338	470	490	236	338	180	1.61	267	313	309	.000					
VARIP Care 19	722	142	894	324	175	400	2.900	1.429	303	.535	31.5	340	297	223	239	236	220	117	.000				
VAR20 Care 20	838	355	350	247	041	334	2.983	1.416	717	465	354	846	118	299	129	023	.036	291	213	.000			
VAR21 Cure 21	817	141	144	.536	352	459	2.366	1.603	363	743	502	402	294	120	447	413	384	268	213	393	000		
VAR22 Care 22	217	222	079	361	177	775	2.990	1.504	336	.583	391	337	200	126	250	197	168	213	096	177	216	000	
VAR23 Core 23	730	210	130	.263	117	.736	2341	1 394	573	481	385	194	835	161	168	179	164	145	020	151	279	107	000

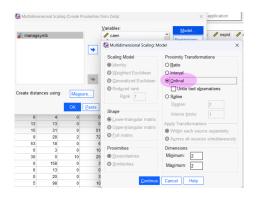
- Another method is that we start with the input of a Distance Matrix
 - lacktriangleright For example, in SPSS, go to Analyze ightarrow Correlate ightarrow Distances.
 - In the dialog box, choose the variables you want to calculate distances for (we select all except the first three variables).
 - ▶ We label the rows by manag



- Select the type of distance measure you want to use (e.g., Euclidean).
 - Click OK to compute the distance matrix. And then export the matrix to an Excel file → Convert to a CSV file and then import this distance matrix



- ullet To conduct non-metric MDS with SPSS, we can still click Analyze o Scale o Multidimensional Scaling (ProxSCAL)....
- In the model, we choose Ordinal Proximity transformation



- It is better to have a distance matrix as input.SPSS does not support many distance functions, we will need to prepare our distance matrix using another software.
 - for example, function vegdist in R library vegan.

License



This work is licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License.