Multidimensional Scaling (MDS)

Contents

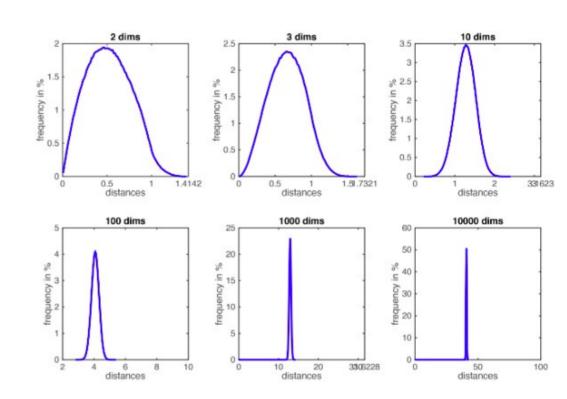
- 1. Dimensionality Reduction
- 2. What is MDS?
- 3. Classical MDS

(Steps, Goodness-of-Fit, Explanations)

4. Non-Metric MDS

Dimensionality Reduction

- ☐ Real data usually have huge number of dimensions. This will cause problems:
 - Data become very sparse, some
 algorithms become meaningless (e.g.
 density based clustering)
 - Several algorithms depend on the dimensionality and they become infeasible (e.g. k-nearest neighbor)



Dimensionality Reduction

- Usually the data can be described with fewer dimensions, without losing much of the meaning of the data.
- ☐ Why reduces dimensions?
 - Discover hidden correlations
 - Remove redundant and noisy features
 - Interpretation and visualization
 - Easier storage and processing of the data

What is MDS?

"Multidimensional scaling (MDS) is a technique for the analysis of **similarity** or **dissimilarity** data on a set of objects. MDS attempts to model such data **as distances among points** in a geometric space.

The main reason for doing this is that one wants a graphical display of the structure of the data, one that is much easier to understand than an array of numbers and, moreover, one that **displays the essential information** in the data, **smoothing out noise**" (Borg and Groenen, 2005).

A **proximity** is a number which indicates how similar or how different two objects are.

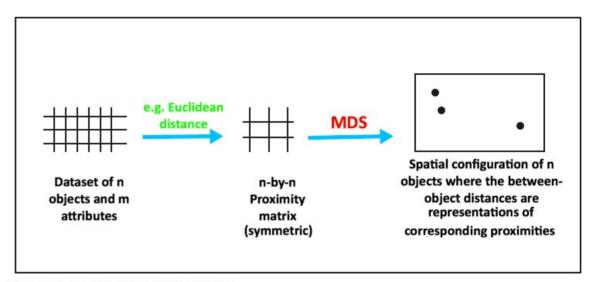


Figure 2- From raw data to MDS configureation

What is MDS?

- \Box The starting point is a matrix of distances or **dissimilarities** between the data points, **D**.
- For example, if we have data on n different experimental units, then we would be given the distances d_{ij} between any pair of experimental units i and j. We compile these into a n × n **distance matrix D** = (d_{ij} : i , j = 1 , ... , n).
- ☐ The goal of MDS is to find a set of points in a low-dimensional Euclidean space R^r , usually R or R^2 or R^3 , whose inter-point distances are as close as possible to the d_{ij} . That is, we want to find $y_1, \dots, y_n \in R^r$ whose distance matrix is approximately D, i.e., for which

$$\operatorname{distance}(\mathbf{y}_i, \mathbf{y}_j) \approx d_{ij}.$$

Y: coordinate matrix

In other words

Find
$$\mathbf{y}_1, \dots, \mathbf{y}_k \in \mathbb{R}^r$$
 to minimize $\sum_{i=1}^n \sum_{j=1}^n (d_{ij} - d(\mathbf{y}_i, \mathbf{y}_j))^2$.

Example. The distance matrix between pairs of cities D:

> real_dist							
	Boston	DC	NY	LA	SC	SF	
Boston	0	439	215	2979	2976	3095	
DC	439	0	233	2631	2684	2799	
NY	215	233	0	2786	2815	2934	
LA	2979	2631	2786	0	384	382	
SC	2976	2684	2815	384	0	87	
SF	3095	2799	2934	382	87	0	

MDS constructs a set of points y_1, \ldots, y_n , that have distances between them given by the distance matrix D. In other words, it creates a map with **a set of coordinates** for which the distances between points are **approximately the same as in the real data**.

Definition 6.1 The $n \times n$ matrix $\mathbf{D} = (d_{ij})_{i,j=1}^n$ is a **distance matrix** (sometimes called a **dissimilarity** matrix) if

- 1. $d_{ij} \geq 0$ for all $i, j = 1, \ldots, n$.
- 2. $d_{ii} = 0$ for i = 1, ..., n and
- 3. $\mathbf{D} = \mathbf{D}^{\top}$, i.e., \mathbf{D} is symmetric ($d_{ij} = d_{ji}$).

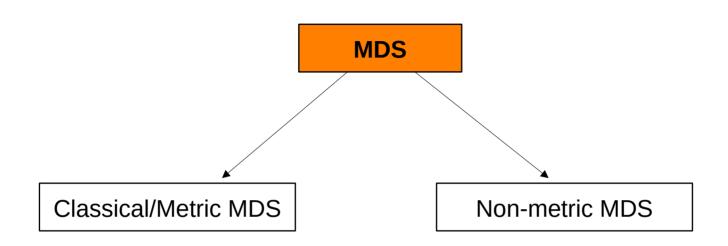
Note that we do not require distances to necessarily satisfy the triangle inequality

$$d_{ik} \le d_{ij} + d_{jk}. \tag{6.2}$$

A distance function which always satisfies the triangle inequality is called a **metric distance** or just a **metric**. A distance function which does not always satisfy the triangle inequality is called a **non-metric** distance.

There are many ways to measure distance. Two common choices of metric distances are

- Euclidean distance $||\mathbf{x} \mathbf{x}'||_2$, also know as the 'crow flies' distance.
- L_1 distance $||\mathbf{x} \mathbf{x}'||_1$, sometimes called the Manhattan or taxicab metric.



- Euclidean distances are usually the first choice for a classical MDS. Since Euclidean distances satisfy the triangle inequality, it follows that Euclidean distance is a metric distance.
- \square The following steps summarize the algorithm of classical MDS:
- 1) Compute nxn distance matrix D
- 2) Calculate the centered inner-product matrix B
- 3) Output coordinate matrix Y by eigenvalue decomposition from B

Package R: cmdscale

Dissimilarity/ — Centering — Centered inner — Coordinate Euclidean matrix D matrix product B matrix Y

1) Compute nxn distance matrix **D**

Definition 6.2 Suppose $\mathbf D$ is an $n \times n$ distance matrix. We say $\mathbf D$ is a **Euclidean distance matrix** if there is a set of points $\mathbf x_1, \dots, \mathbf x_n \in \mathbb R^p$ for some p, such that

$$d_{ij} = ||\mathbf{x}_i - \mathbf{x}_j||_2 = \sqrt{(\mathbf{x}_i - \mathbf{x}_j)^{ op}(\mathbf{x}_i - \mathbf{x}_j)}.$$

Proximity matrix

> real_	dist					
	Boston	DC	NY	LA	SC	SF
Boston	0	439	215	2979	2976	3095
DC	439	0	233	2631	2684	2799
NY	215	233	0	2786	2815	2934
LA	2979	2631	2786	0	384	382
SC	2976	2684	2815	384	0	87
SF	3095	2799	2934	382	87	0

Euclidean distance matrix/ Dissimilarity matrix





2) Calculate the centered inner-product matrix B

Definition 6.3 Given a distance matrix $\mathbf{D} = \{d_{ij}\}_{i,j=1}^n$, the **centred inner-product matrix** (also called the **centred-Gram matrix**) is

$$\mathbf{B} = \mathbf{H}\mathbf{A}\mathbf{H},\tag{6.3}$$

where ${f A}$ is the matrix of negative square distances divided by two:

$$\mathbf{A} = \{a_{ij}\}_{i,j=1}^n, \text{ where } a_{ij} = -\frac{1}{2}d_{ij}^2$$
 (6.4)

H is the n × n centering matrix: $H = I_n - n^{-1}J_n$

$$d_{ij}^{2}$$

$$a_{ij}=-rac{1}{2}d_{ij}^2$$

> D^2						
	Boston	DC	NY	LA	SC	SF
Boston	0	679750	223977	43242620	45295266	47211341
DC	679750	0	218165	37945620	39914758	41820949
NY	223977	218165	0	41336157	43353985	45316668
LA	43242620	37945620	41336157	0	385596	443641
SC	45295266	39914758	43353985	385596	0	56689
SF	47211341	41820949	45316668	443641	56689	0

$$H = I_n - n^{-1}J_n$$

1	0	0	0	0	0
0	1	0	0	0	0
0	0	1	0	0	0
0	0	0	1	0	0
0	0	0	0	1	0
0	0	0	0	0	1

- 1/6 *

$$H = I_n - n^{-1}J_n$$

```
<- H%*%A%*%H
> B
         [,1]
                  [,2]
                             [,3]
                                      [,4]
                                                [,5]
                                                          [,6]
[1,]
     12013126
               10333775 11384138 -10716460 -11271728 -11742850
     10333775
              9334174 10047568
[2,]
                                  -9407436
                                             -9920950 -10387130
[3,]
     11384138 10047567 10979126 -10280229 -10818088 -11312514
    -10716461
               -9407436 -10280229
                                            10074830
                                  9796573
                                                      10532724
[5,] -11271728
               -9920951 -10818088
                                 10074830
                                            10738683
                                                      11197254
    -11742850 -10387130 -11312513
                                  10532724
                                            11197254
                                                      11712515
```

B the centered inner-product matrix. The inner product is large if x_i is similar to x_j , and small if they are very different

3) Output coordinate matrix Y by eigenvalue decomposition from B

Suppose B has eigenvalues $\lambda 1 \ge \lambda 2 \cdots \ge \lambda k > 0$ and that it has **spectral decomposition**

$$B = U\Lambda U^{T}$$

 $\Lambda = \text{diag}\{\lambda 1...\lambda k\}$ and U is the nxk matrix of k eigenvalues

(Keep only **few largest eigenvalues k** and corresponding eigenvectors)

Then coordinate matrix Y:

$$Y = [y1, ..., yn]^T = U \Lambda^{1/2}$$

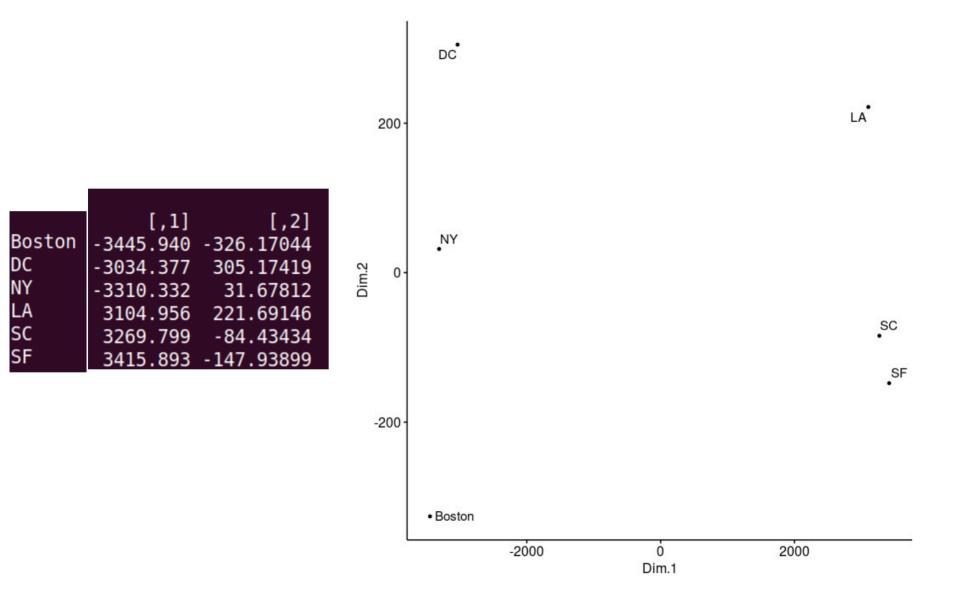
```
eigen(B)
eigen() decomposition
$values
    6.404091e+07 2.786842e+05 2.111650e+05 3.172240e+04 1.171405e+04
[6] -6.510788e-10
$vectors
                                                           [,5]
           [,1]
                       [,2]
                                   [,3]
                                               [,4]
                                                                      [,6]
[1,] -0.4306048 -0.61785770 -0.37012528
                                         0.29981747
                            0.35381850
                                        -0.75244055 -0.29755897 -0.4082483
                            0.06253239
                0.41994539
                            -0.71064324 -0.02756709
                                                    0.02578586 -0.4082483
     0.4085944 -0.15994217
                            0.39612371 -0.24101166
                                                    0.65253496 -0.4082483
                                        0.24873026 -0.66238257 -0.4082483
     0.4268503 -0.28023766 0.26829393
                  u2
      u1
```

[,1] [,2] [1,] 8002.557 0.0000 [2<u>,</u>] 0.000 527.9054

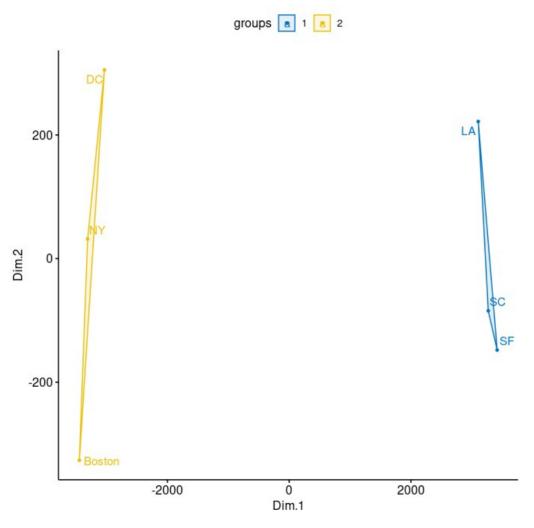
sqrt(λ1)	0
0	sqrt(λ2)

_

$$Y = U \Lambda^{1/2}$$



Cluster by k-means



Classical MDS: Goodness-of-Fit

```
> Y.mds
$points
                     [,2]
           [,1]
Boston -3445.940 326.17044
       -3034.377 -305.17419
      -3310.332 -31.67812
      3104.956 -221.69146
    3269.799
                84,43434
      3415.893 147.93899
$eig
[1] 6.404091e+07 2.786842e+05 2.111650e+05 3.172240e+04 1.171405e+04
[6] -2.229196e-09
$x
NULL
$ac
[1] 0
$G0F
[1] 0.9960572 0.9960572
```

Classical MDS: Goodness-of-Fit

P, value

- □P2 value is computed as the sum of the eigenvalues for the number of dimensions divided by the total sum of the eigenvalues.
- The eigenvalue is a measure of the generalized variance, so **P2 indicates the amount of generalized variance explained by the dimensions out of the total variance** in the
 matrix.
- ☐ The P2 values range from 0 to 1 with values closer to 1 indicating a better fit.
- \square If there are two dimensions, the P2 value is computed as follows:

$$P_2 = \frac{\Sigma(\lambda_1 + \lambda_2)}{\Sigma \lambda_{y}}.$$

Classical MDS: Goodness-of-Fit

Mardia criterion

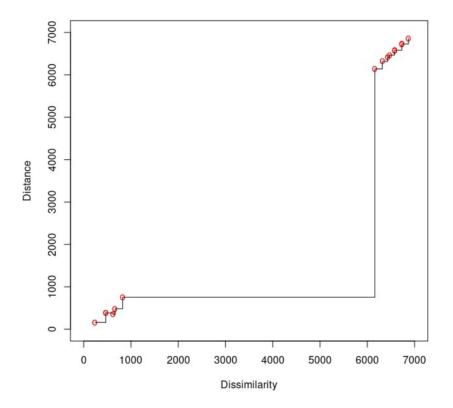
- ☐ Mardia criterion is a variation on P2.
- ☐ Mardia values range from 0 to 1 with values closer to 1 indicating a better model fit.
- ☐ The Mardia value for a two dimension solution would be computed as follows:

Mardia =
$$\frac{\Sigma(\lambda_1^2 + \lambda_2^2)}{\Sigma \lambda_N^2}.$$

Classical MDS: Shepard diagram

Show the connection between distance from coordinate matrix Y and Euclidean distance

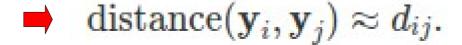
(dissimilarity)



The coordinate values for each city do not fall far from the line \rightarrow a good model fit

```
> D <- as.matrix(dist(real dist, upper=T, diag=T))</pre>
> D
                                   NY
                                                        SC
          Boston
                         DC
                                             LA
          0.0000
                  824.4695
                            473, 2621 6575, 9121 6730, 1758 6871, 0509
Boston
        824.4695
                     0.0000
                             467.0814 6160.0016 6317.8128 6466.9119
DC
NY
        473.2621
                  467.0814
                               0.0000 6429.3201 6584.3743 6731.7656
LA
       6575.9121 6160.0016 6429.3201
                                         0.0000
                                                 620.9638
                                                            666.0638
       6730.1758 6317.8128 6584.3743
                                       620.9638
                                                    0.0000
                                                            238.0945
       6871.0509 6466.9119 6731.7656
                                      666.0638
                                                 238.0945
                                                              0.0000
```

```
signif(dist(Y, upper=T, diag=T))
          753.645
                   382.681 6573.770 6720.090 6864.150
                   388.524 6139.900 6316.200 6466.170
 753.645
            0.000
 382.681
          388.524
                     0.000 6418.100 6581.160 6728.620
6573.770 6139.900 6418.100
                              0.000
                                     347.687
                                              483.020
6720.090 6316.200 6581.160
                            347.687
                                        0.000
                                               159.299
6864.150 6466.170 6728.620
                            483.020
                                      159.299
                                                 0.000
```



Similarity between vector a (SC) and b (SF)

$$a = [a1 \ a2 \ ... \ an], \qquad b = [b1 \ b2 \ ... \ bn]$$

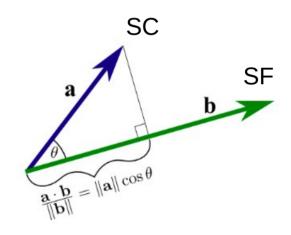
$$a.b = a1b1 + a2b2 + ... + anbn = \Sigma aibi$$

This dot product a·b should depend on the magnitude of both vectors, $\|\mathbf{a}\|$ and $\|\mathbf{b}\|$.

It reflects both magnitude and direction

=> The inner product is **large if a is similar to b**, and

small if they are very different



Dissimilarity/ Euclidean matrix D



Centering matrix



Centered inner product B

(1)



Euclidean distance between a and b

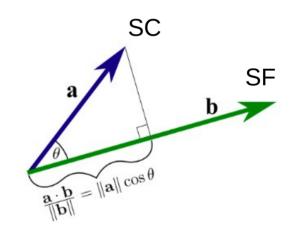
$$\Sigma(ai - bi)^2 = \Sigma(ai^2 + bi^2 - 2aibi) = \Sigma(ai)^2 + \Sigma(bi)^2 - 2\Sigma(aibi)$$

Inner product

Replace coordinate matrix Y to (1) (Y preserves the real distance)



SC/a SF/b 3269.799 -84.43434 3415.893 -147.93899



Dissimilarity/ Centering — Centered inner — Euclidean matrix D matrix product B

 $+ \Sigma$

$$D^{2}(Y) = \sum \frac{y_{a}^{2}}{y_{b}^{2}} \frac{y_{a}^{2}}{y_{b}^{2}}$$

y ² _a	y ² _b
y _a	y ² _b

$y_{a1}y_{a1} + y_{a2}y_{b1}$	$y_{a1}y_{a2} + y_{a2}y_{b2}$
$y_{b1}y_{a1} + y_{b2}y_{b1}$	$y_{b1}y_{a2} + y_{b1}y_{b2}$

$$= c1' + 1c' - 2YY'$$
 $= c1' + 1c' - 2B$

Y

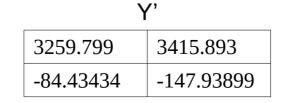
3269.799 -84.43434 3415.893 -147.93899

SC/a

SF/b

34 99

X



10738683 11197254 11197254 11712515

Coordinate

matrix Y

$$H = I_n - n^{-1}J_n = I_n - n^{-1}11'$$

$$B = HAH = -1/2* H D^2 H = -1/2* H (c1' + 1c' -2B) H$$

$$= HBH = B$$

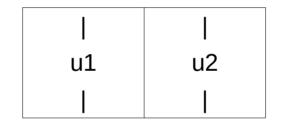
centering a vector of ones yields a vector of zeros

The centering around B can be removed because B is centered

$$Bu_1 = \lambda_1 u_1$$

$$Bu_2 = \lambda_2 u_2$$

B u1 u2



λ1	0
0	λ2

$$BU = U\Lambda$$

$$B = U \Lambda U^{-1}$$

$$U \wedge U^{-1} = (U \wedge^{1/2})(U \wedge^{1/2})' = B = YY'$$

Non-Metric MDS

The assumption that proximities behave like distances might be too restrictive.

Metric vs. Non-metric

Proximity Matrix: Assign a numerical value to indicate the distance between pairs of objects

- Real distances between cities (metric)
- Rank of cities (non-metric)

Non-Metric MDS

The non-metric MDS approach uses ordinal data

For example, how do you rank these pictures from simple to complex drawing?

1: very simple → 10: very complex



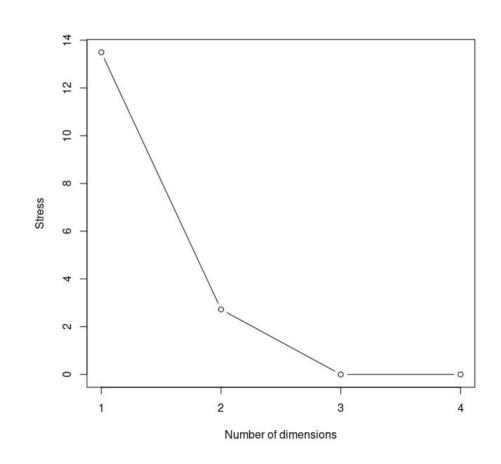
Non-metric MDS finds a low-dimensional representation, which respects the ranking of distances

Non-Metric MDS: Stress

STRESS =
$$\sqrt{\frac{\sum (f(p) - d)^2}{\sum d^2}}$$
.

p is the proximitiesd is the point distancesf(p) is scaled proximities

Goal: minimizes the squared differences between the optimally scaled proximities and the distances between the points



Non-Metric MDS: Stress

Judging the goodness of fit

The amount of stress may also be used for judging the goodness of fit of an MDS solution: a small stress value indicates a good fitting solution, whereas a high value indicates a bad fit. Kruskal (1964a) provided some guidelines for the interpretation of the stress value with respect to the goodness of fit of the solution (Table 2).

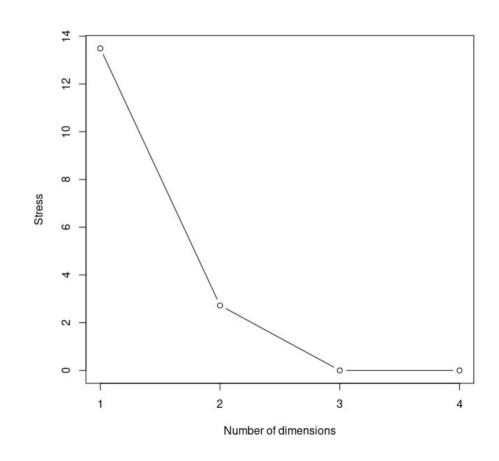
Stress	Goodness of fit
> .20	poor
.10	fair
.05	good
.025	excellent
.00	perfect

Table 2: Stress and goodness of fit.

Stress decreases as the number of dimensions increases. Thus, a two-dimensional solution always has more stress than a three-dimensional one

Non-Metric MDS: Scree plot

In a scree plot, the amount of stress is plotted against the number of dimensions. Since stress decreases with increasing dimensionality, one is looking for the lowest number of dimensions with acceptable stress.



Non-Metric MDS

The following steps summarize the algorithm of non-metric MDS:

- 1) Compute correlation matrix
- 2) Compute nxn distance matrix D
- 3) Calculate the centered inner-product matrix B
- 4) Output coordinate matrix Y by eigenvalue decomposition from B
- 5) Compare the stress to some criterion. If the stress is small enough then exit the algorithm else choose another number of dimensions and run again

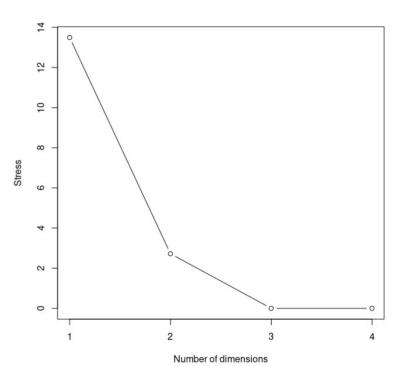
Example

>	dat						
	Sample	Species.1	Species.2	Species.3	Species.4	Species.5	Species.6
1	1	46	72	7	13	9	142
2	2	51	124	5	16	3	49
3	3	23	44	3	6	2	16
4	4	12	41	1	18	4	21
5	5	4	40	0	19	6	10
6	6	23	16	2	13	0	6
7	7	46	33	19	27	11	31

The similarity between two species means that they account for the same proportion in each sample group

```
> signif(dist(Y2, upper=T, diag=T))
          Species.1 Species.2 Species.3 Species.4 Species.5 Species.6
Species.1 0.0000000 0.9125900 0.9085760 0.9440290 0.9376470 1.0031300
Species.2 0.9125900 0.0000000 1.5997000 1.8533900 1.6222400 0.9762570
Species.3 0.9085760 1.5997000 0.0000000 0.9802880 0.0297536 0.9856680
Species.4 0.9440290 1.8533900 0.9802880 0.0000000 1.0006900 1.7328400
Species.5 0.9376470 1.6222400 0.0297536 1.0006900 0.0000000 0.9931410
Species.6 1.0031300 0.9762570 0.9856680 1.7328400 0.9931410 0.0000000
> signif(dist(Y3, upper=T, diag=T))
          Species.1 Species.2 Species.3 Species.4 Species.5 Species.6
Species.1
          0.000000 0.906444 0.706195 1.291670
                                                 1.028890
                                                            0.875201
Species.2 0.906444
                    0.000000
                             1.400120 1.471960
                                                 1.390920
                                                            0.979028
Species.3
           0.706195
                    1.400120
                              0.000000
                                        0.858727
                                                  0.689664
                                                            1.193820
Species.4 1.291670
                    1.471960
                              0.858727
                                        0.000000
                                                  0.828554
                                                            1.535370
Species.5 1.028890
                    1.390920
                              0.689664 0.828554 0.000000
                                                            0.916426
Species.6 0.875201
                              1.193820
                                        1.535370
                                                  0.916426
                                                            0.000000
                    0.979028
> dist nmds
          Species.1 Species.2 Species.3 Species.4 Species.5 Species.6
Species.1 0.0000000 0.8975582 0.7919713 1.3067679 1.1113227 0.8857866
Species.2 0.8975582 0.0000000 1.4140676 1.4836935 1.3928624 1.0210047
Species.3 0.7919713 1.4140676 0.0000000 0.8838707 0.7300773 1.2282366
Species.4 1.3067679 1.4836935 0.8838707 0.0000000 0.8285425 1.4854911
```

Species.5 1.1113227 1.3928624 0.7300773 0.8285425 0.0000000 0.9922403 Species.6 0.8857866 1.0210047 1.2282366 1.4854911 0.9922403 0.0000000



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