Columbidae University

Final year project

Pigeons love doves

John Birdwatch

supervised by
Dr. Mark Brown

December 15, 2018

Contents

Chapter 1

Classical Multidimensional Scaling

1.1 The basic ideas of Multidimensional Scaling

Multidimensional Scaling (MDS) is a method that represents measurements of similarity (or dissimilarity) among pairs of objects as distances between points of a low-dimensional multidimensional space. The data, for example, may be correlations among intelligence test, and the MDS representation is a plane that shows the tests as points that are closer together the more positively the tests are correlated. The graphical display of the correlations provided by MDS enables the data analyst to literally "look" at the data and to explore the structure visually. This often shows regularities that remain hidden when studying arrays of numbers. Another application of MDS is to use some of its mathematical as models for dissimilarities judgements. For example, given two objects of interest, one may explain their perceived dissimilarity as the result of a mental arithmetic that mimics the distance formula. According to this model, the mind generates impression of dissimilarity by adding up the perceived differences of the two objects over this properties.

Given a square matrix $\mathbf{D}$ $n \times n$, the goal of MDS is to obtain a set of orthogonal variables $y_1, ..., y_p$, which are called *principal coordinates*, where $p < n$, such that the Euclidean distances of the elements with respect of these variables are equal to the matrix $\mathbf{D}$. Therefore, the aim is to obtain a matrix $\mathbf{X}$ $n \times p$ that could be interpreted as the matrix of p variables for the n observations , where the Euclidean distance between the elements could be approximated by $\mathbf{D}$.

This approach arises two questions: is it (always) possible to find these variables? How are they obtained? In general, it is not possible to find a set of p variables that reproduces *exactly* the initial distance. However, it is possible to find a set of variables which distance is approximately the initial distance matrix $\mathbf{D}$.

As a classic example, consider the distances between European cities as in the table 1.1. One would like to get a representation in a 2-dimensional space such that the distances were almost the same as in table 1.1. MDS is able to build an embedding into a 2-dimensional space. The representation of these corrdinates are displayed in figure 1.1.

Quetelet made an effort trying to quantify some experiments made in the social sciences, but it can be considered that MDS was born in the 50th century when experimental pschycologists wanted to discover similarities between applied to different

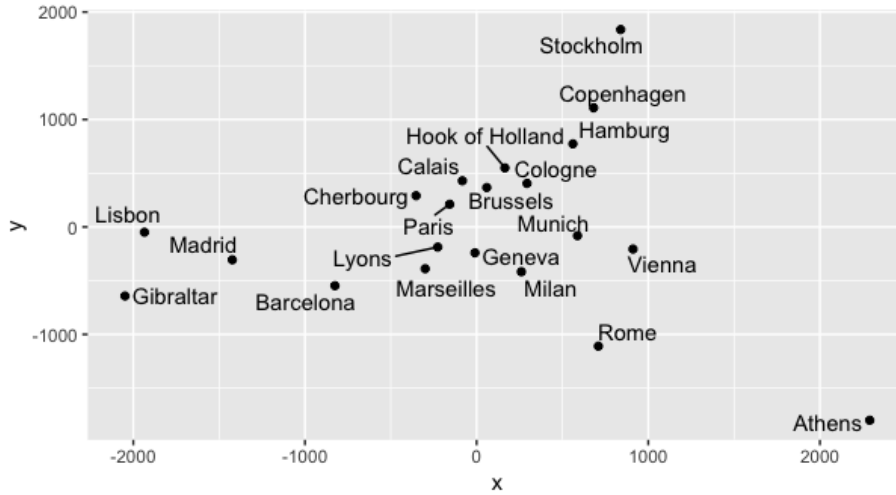|	Athens	Barcelona	Brussels	Calais	Cherbourg
Athens	0.00	3313.00	2963.00	3175.00	3339.00
Barcelona	3313.00	0.00	1318.00	1326.00	1294.00
Brussels	2963.00	1318.00	0.00	204.00	583.00
Calais	3175.00	1326.00	204.00	0.00	460.00
Cherbourg	3339.00	1294.00	583.00	460.00	0.00

Table 1.1: Distances between European cities

Figure 1.1: MDS on the Eurepean cities.

people.

MDS methods can be divided into two groups: *Metric MDS* and *Non-metric MDS*. Metric MDS, also known as principal coordinates, use the differences between similarities. However, Non-metric MDS states that if a is more similar to b than c, then a is closer to b than c, but the differences between the similarities ab and ac do not have any interpretation.

1.2 A historical Account

The first decade was pioneered by the seminal work of Torgerson (1952), he defined the multidimensional scaling problem and provided the first metric solution.

- Torgerson[1] provided the first complete explication of a MDS method. Although Klingberg (1941) had already performed a "crude" MDS scaling of data concerning the degree of hostility between nations, the first systematic procedure for determining the MDS map of points from errorful interpoint distances was provided by Torgerson (1952)[1].

- This process introduced three major steps:

    - A scale of comparative distances between all pairs of stimuli is obtained (i.e. measured on an interval scale)

– Distances between each pair of stimuli are located on a distance continuum. In paired comparisons, the procedures for obtaining a scale of comparative distances leave the true zero point undetermined. A comparative distance is not a distance in the usual sense of the term, but is a distance minus an unknown constant. When the unknown constant is obtained, the comparative distances can be converted into absolute (i.e., ratio) distances.

– The dimensionality of the psychological space necessary to account for these absolute distances is determined, and the projections of stimuli on axes of this space are obtained.

The second decade of work was heralded in by the innovative work of Shepard (1962)[2] and Kruskal (1964)[3] on non-metric multidimensional scaling, and saw the highly illuminating work of Coombs (1964)[4] on data theory.

- This very active decade included work that focused on developing methods for analyzing ordinal dissimilarities data known as nonmetric MDS. This stage became popularized by Shepard (1962)[2] who turned "MDS from a data analysis procedure familiar to a few aficionados into a procedure used in such diverse disciplines as architecture and zoology, geography and political science, and psychology and business administration.". Shepard pointed out the idea that one could recover metric information from nonmetric information.

The third decade included 25 years of developments by Takane, Young, and De Leeuw (1976)[5], and by the De Leeuw and Heiser (1980)[6]. The trend setting work came from Carroll and Chang (1970)[7] on individual differences MDS.

- Before this point, MDS procedures could only analyze a single matrix of data. Leading to the development of "individual differences" MDS. (i.e. procedures that were able to simultaneously analyze a number of data matrices without the necessity of any type of averaging process).

- Carroll and Chang proposed a model for representing cognitive/perceptual individual differences whose psychological appeal was very high, which displayed individual differences in an easily assimilated and parsimonious fashion.

The fourth decade presented the development of constrained MDS and maximum likelihood multidimensional scaling, as exemplified by Ramsay (1982) and Takane (1980a, 1980b)[5].

- Constrained MDS - introduction of constraints on the parameters of the model.

- Maximum likelihood MDS - A maturing of the data analysis technology usually brings a desire for an explanation of the error model involved in the fitting process (Ramsay 1977).

- This approach changes MDS from a descriptive tool into an inferential tool.

- This includes the development of significant tests to determine the appropriate dimensionality, appropriate MDS model, and appropriate error model.

- This approach provides confidence regions for the stimuli and with weighted models for subjects.

Most applications of MDS today actually serve a wide purpose, i.e. they are done to visualize tables of indices that can be interpreted as (dis)similarity data. For that purpose, MDS is highly useful as it can handle a vast variety of data as long as they are (dis)similarities (e.g., correlations, covariances, co-occurrence data, profile distances).

1.3 Principal coordinates

Given a Matrix $\mathbf{X}$ $n \times p$, one can interpret it as the matrix of n individuals over p variables. It is easy to see that the following matrix has mean zero:

$$\widetilde{\mathbf{X}} = \left(\mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}'\right) = \mathbf{P}\mathbf{X}$$

This new matrix, $\widetilde{\mathbf{X}}$ has the same dimensions as the orginial one, but it is centered. From this matrix, it is possible to build two square semi-positive definite matrices: the covariance matrix $\mathbf{S}$, defined as $\widetilde{\mathbf{X}}'\widetilde{\mathbf{X}}/n$ and the cross-prodructs matrix $Q = \widetilde{\mathbf{X}}\widetilde{\mathbf{X}}'$. This matrix can be interpred as a similarity matrix between the n elements. The term ij is obtained as follows:

$$q_{ij} = \sum_{s=1}^{p} x_{is}x_{js} = \mathbf{x_i}'\mathbf{x_j} \tag{1.1}$$

where $\mathbf{x_i}'$ is the i-th row from $\widetilde{\mathbf{X}}$. Given the scalar product formula, $\mathbf{x_i}'\mathbf{x_j} = \mid \mathbf{x_i} \mid\mid \mathbf{x_i} \mid cos\theta_{ij}$, if the elements i and j have similar coordinates, then $cos\theta_{ij} \simeq 1$ and q_{ij} will be large. On the contrary, if the elements are very different, then $cos\theta_{ij} \simeq 0$ and q_{ij} will be small. So, $\widetilde{\mathbf{X}}\widetilde{\mathbf{X}}'$ can be interpreted as the similarity matrix between the elements.

The distances between elements can be deduced from the similarity matrix. The euclidean distance between to elements is calculated in the following way:

$$d_{ij}^2 = \left(\sum_{s=1}^{p} x_{is} - x_{js}\right)^2 = \sum_{s=1}^{p} x_{is}^2 + \sum_{s=1}^{p} x_{js}^2 - 2\sum_{s=1}^{p} x_{is}x_{js} \tag{1.2}$$

This expression can be obtained directly from the matrix $\mathbf{Q}$:

$$d_{ij}^2 = q_{ii} + q_{jj} - 2q_{ij} \tag{1.3}$$

We have seen that given the matrix $\widetilde{\mathbf{X}}$, it is possible to get the similarity matriz $\mathbf{Q} = \widetilde{\mathbf{X}}\widetilde{\mathbf{X}}'$ and from it, to get the distance matrix $\mathbf{D}$. Let $diag(\mathbf{Q})$ be the vector that contains the diagonal terms of $\mathbf{Q}$ and $\mathbf{1}$ be the vector of ones, the matrix $\mathbf{D}$ is given by:

$$\mathbf{D} = diag(\mathbf{Q})\mathbf{1}' + \mathbf{1}diag(\mathbf{Q})' - 2\mathbf{Q}$$

The problem we are dealing with goes in the opposite direction. We want to rebuid $\widetilde{\mathbf{X}}$ from a square distance matrix $\mathbf{D}$, with elements d_{ij}^2. The first step is to obtain $\mathbf{Q}$ and afterwards, to get $\widetilde{\mathbf{X}}$.

The first step is to find out a way to obtain the matrix $\mathbf{Q}$ given $\mathbf{D}$. We can assume without loss of generality that the mean of the variables is equal to 0. This is a consequence of the fact that the distance between two points keeps unchanged if the variables are expressed in terms of the mean:

$$d_{ij}^2 = \sum_{s=1}^{p} (x_{is} - x_{js})^2 = \sum_{s=1}^{p} [(x_{is} - \overline{x_s}) - (x_{js} - \overline{x_s})]^2 \qquad (1.4)$$

The previous condition means that we are lookig for a matrix $\widetilde{\mathbf{X}}$ such that $\widetilde{\mathbf{X}}'\mathbf{1} = 0$. It also means that $\mathbf{Q1} = 0$, i.e, the sum of all the elements of a row of $\mathbf{Q}$ is 0. Since the matrix is symmetric, the previous condition should state for the columns as well.

To establish this constrains, we sum up 1.2 at row level:

$$\sum_{i=1}^{n} d_{ij}^2 = \sum_{i=1}^{n} q_{ii} + nq_{jj} = t + nq_{jj} \qquad (1.5)$$

where $t = \sum_{i=1}^{n} q_{ii} = trace(\mathbf{Q})$, and we have used that the condition $\mathbf{Q1} = 0$ implies $\sum_{i=1}^{n} q_{ij} = 0$. Summing up the 1.2 at column level:

$$\sum_{i=1}^{n} d_{ij}^2 = t + nq_{ii} \qquad (1.6)$$

Summing up 1.5 we obtain:

$$\sum_{i=1}^{n} \sum_{j=1}^{n} d_{ij}^2 = 2nt \qquad (1.7)$$

Replacing in 1.3 q_{jj} obtained in 1.5 and q_{ii} obtained in 1.6, we have the following expression:

$$d_{ij}^2 = \frac{1}{n} \sum_{i=1}^{n} d_{ij}^2 - \frac{t}{n} + \frac{1}{n} \sum_{j=1}^{n} d_{ij}^2 - \frac{t}{n} - 2q_{ij} \qquad (1.8)$$

Let $d_{i.}^2 = \frac{1}{n} \sum_{j=1}^{n} d_{ij}^2$ and $d_{.j}^2 = \frac{1}{n} \sum_{i=1}^{n} d_{ij}^2$ be the row-mean and column-mean. Using 1.7, we have that:

$$d_{ij}^2 = d_{i.}^2 + d_{.j}^2 - d_{..}^2 - 2q_{ij} \qquad (1.9)$$

where $d_{..}$ if the mean of all the elements of $\mathbf{D}$, gven be:

$$d_{..}^2 = \frac{1}{n^2} \sum \sum d_{ij}^2$$

Finally, from 1.9 we get the following expression:

$$q_{ij} = -\frac{1}{2}(d_{ij}^2 - d_{i.}^2 - d_{.j}^2 + d_{..}^2) \qquad (1.10)$$

The previous expression shows how to build the matrix of similarities $\mathbf{Q}$ from the distance matrix $\mathbf{D}$.

The next step is to obtain the matrix $\mathbf{X}$ given the matrix $\mathbf{Q}$. Let's supose that the similarity matrix es positive definite of range p, it can be represented by

$$\mathbf{Q} = \mathbf{V\Lambda V}'$$

where $\mathbf{V}$ is a $n \times p$ matrix that contains the eigenvectors with eigenvalues not nulls of $\mathbf{Q}$, $\mathbf{\Lambda}$ is a diagonal matrix $p \times p$ that contains the eigenvalues.

Re-writing the previous expression, we obtain:

$$\mathbf{Q} = (\mathbf{V}\mathbf{\Lambda}^{1/2})(\mathbf{\Lambda}^{1/2}\mathbf{V}') \tag{1.11}$$

Getting:

$$Y = \mathbf{V}\mathbf{\Lambda}^{1/2}$$

we have obtained a matrix with dimesions $n \times p$ with p uncorrelated variables that reproduces the initial metric. It is important to notice that if one starts from $\mathbf{X}$ (i.e $\mathbf{X}$ is known) and calculates from these variables the distance matrix in 1.2 and after that it is applied the method explained, the matrix obtained is not the same as $\mathbf{X}$, but its principal components. This happens since the distance between elements does not change if:

- The mean values are modified

- Poits are rotated, i.e, multiplications by orthogonal matrices

By 1.3, the distance is a function of the terms of the similarity matrix $\mathbf{Q}$ and this matrix is invariant given any rotations of the variables:

$$\mathbf{Q} = \widetilde{\mathbf{X}}\widetilde{\mathbf{X}'} = \widetilde{\mathbf{X}}\mathbf{A}\mathbf{A}'\widetilde{\mathbf{X}'}$$

for any orthogonal $\mathbf{A}$ matrix. The matrix $\mathbf{Q}$ anly contains information about the space generated by the variables $\mathbf{X}$. Any rotation keeps the distance unchaged. As a consequence, any rotation of the original variables could be a valid solution.

1.4 Building principal coordinates

1.5 Procrustes transformation

Chapter 2

Divde and Conquer Multidimensional Scaling

Chapter 3

Fast Multidimensional Scaling

Chapter 4

Multidimensional Scaling based on Gower interpolation formula

Chapter 5

Simulation study

Chapter 6

Conclusions

Bibliography

[1] Warren S. Torgerson. Multidimensional scaling: I. theory and method. *Psychometrika*, 17(4):401–419, Dec 1952.

[2] Roger N. Shepard. The analysis of proximities: Multidimensional scaling with an unknown distance function. ii. *Psychometrika*, 27(3):219–246, Sep 1962.

[3] J. B. Kruskal. Nonmetric multidimensional scaling: A numerical method. *Psychometrika*, 29(2):115–129, Jun 1964.

[4] C. H. Coombs. *A theory of data*. Wiley, New York, 1964.

[5] Yoshio Takane, Forrest W. Young, and Jan De Leeuw. nonmetric common factor analysis: an alternating least squares method with optimal scaling features. *Behaviormetrika*, 6:45–56, Jan 1979.

[6] Jan De Leeuw and Willem Heiser. Multidimensional scaling with restrictions on the configuration. *Multivariate Analysis*, 5, Jan 1980.

[7] J. Douglas Carroll and Jih-Jie Chang. Analysis of individual differences in multidimensional scaling via an n-way generalization of "eckart-young" decomposition. *Psychometrika*, 35(3):283–319, Sep 1970.

[8] Ingwer Borg and Patrick Groenen. *Modern Multidimensional Scaling*. Springer-Verlag, New York, NY, 1997.

[9] Daniel Peña. *Análisis de datos multivariantes*. McGraw Hill, Madrid, Spain, 2002.

[10] Patrick Groenen and Ingwer Borg. The past, present, and future of multidimensional scaling, Jan 2013.

[11] Ernst Z. Rothkopf. A measure of stimulus similarity and errors in some paired-associate learning tasks. *Journal of Experimental Psychology*, 53(2):94, 1957.

Appendix A

masblablabl

blabla