Multidimensional Scaling

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Abstract

Multidimensional scaling is a statistical technique to visualize dissimilarity data. In multidimensional scaling, objects are represented as points in a usually two dimensional space, such that the distances between the points match the observed dissimilarities as closely as possible. Here, we discuss what kind of data can be used for multidimensional scaling, what the essence of the technique is, how to choose the dimensionality, transformations of the dissimilarities, and some pitfalls to watch out for when using multidimensional scaling.

1   Introduction

Multidimensional scaling is a statistical technique originating in psychometrics. The data used for multidimensional scaling (MDS) are dissimilarities between pairs of objects. The main objective of MDS is to represent these dissimilarities as distances between points in a low dimensional space such that the distances correspond as closely as possible to the dissimilarities.

Let us introduce the method by means of a small example. Ekman (1954) collected data to study the perception of 14 different colors. Every pair of colors was judged by a respondent from having 'no similarity' to being 'identical'. The obtained scores can be scaled in such a way that identical colors are denoted by 0, and completely different colors by 1. The averages of these dissimilarity scores over the 31 respondents are presented in Table 1. Starting from wavelength 434, the colors range from bluish-purple, blue, green, yellow, to red. Note that the dissimilarities are symmetric: the extent to which colors with wavelengths 490 and 584 are the same is equal to that of colors 584 and 490. Therefore, it suffices to only present the lower triangular part of the data in Table 1. Also, the diagonal is not of interest in MDS because the distance of an object with itself is necessarily zero.

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Table 1: Dissimilarities of colors with wavelengths from 434 to 674 nm (Ekman, 1954).

nm	434	445	465	472	490	504	537	555	584	600	610	628	651	674
434	–													
445	.14	–												
465	.58	.50	–											
472	.58	.56	.19	–										
490	.82	.78	.53	.46	–									
504	.94	.91	.83	.75	.39	–								
537	.93	.93	.90	.90	.69	.38	–							
555	.96	.93	.92	.91	.74	.55	.27	–						
584	.98	.98	.98	.98	.93	.86	.78	.67	–					
600	.93	.96	.99	.99	.98	.92	.86	.81	.42	–				
610	.91	.93	.98	1.00	.98	.98	.95	.96	.63	.26	–			
628	.88	.89	.99	.99	.99	.98	.98	.97	.73	.50	.24	–		
651	.87	.87	.95	.98	.98	.98	.98	.98	.80	.59	.38	.15	–	
674	.84	.86	.97	.96	1.00	.99	1.00	.98	.77	.72	.45	.32	.24	–

MDS tries to represent the dissimilarities in Table 1 in a map. Figure 1 presents such an MDS map in 2 dimensions. We see that the colors, denoted by their wavelengths, are represented in the shape of a circle. The interpretation of this map should be done in terms of the depicted inter-point distances. Note that, as distances do not change under rotation, a rotation of the plot does not affect the interpretation. Similarly, a translation of the solution (that is, a shift of all coordinates by a fixed value per dimension) does not change the distances either, nor does a reflection of one or both of the axes.

Figure 1 should be interpreted as follows. Colors that are located close to each other are perceived as being similar. For example, the colors with wavelengths 434 (violet) and 445 (indigo) or 628 and 651 (both red). In contrast, colors that are positioned far away from each other, such as 490 (green) and 610 (orange) indicate a large difference in perception. The circular form obtained in this example is in accordance with theory on the perception of colors.

Summarizing, MDS is a technique that translates a table of dissimilarities between pairs of objects into a map where distances between the points match the dissimilarities as well as possible. The use of MDS is not limited to psychology but has applications in a wide area of disciplines, such as sociology, economics, biology, chemistry, and archaeology. Often, it is used as a technique for exploring the data. In addition, it can be used as a technique for dimension reduction. Sometimes, as in chemistry, the objective is to reconstruct a 3D model for large DNA-molecules for which only partial information of the distances between atoms is available.
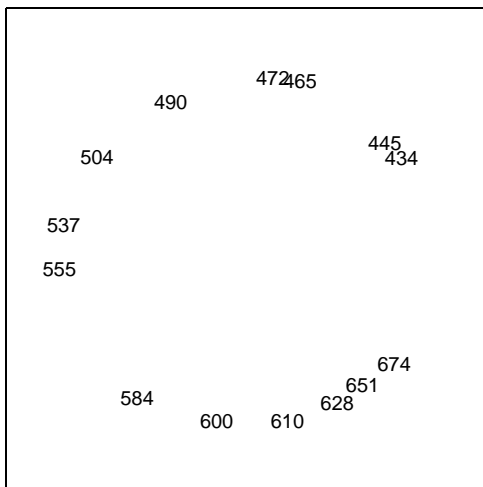
472 465

490

445
504 434

537

555

674
651
584 628
600 610

Figure 1: MDS solution in 2 dimensions of the color data in Table 1.

2   Data for MDS

In the previous section, we introduced MDS as a method to describe relationships between objects on the basis of observed dissimilarities. However, instead of dissimilarities we often observe similarities between objects. Correlations, for example, can be interpreted as similarities. By converting the similarities into dissimilarities MDS can easily be applied to similarity data. There are several ways of transforming similarities into dissimilarities. For example, we may take one divided by the similarity or we can apply any monotone decreasing function that yields nonnegative values (dissimilarities cannot be negative). However, in Section 4, we shall see that by applying transformations in MDS, there is no need to transform similarities into dissimilarities. To indicate both similarity and dissimilarity data, we use the generic term proximities.

Data in MDS can be obtained in a variety of ways. We distinguish between the direct collection of proximities versus derived proximities. The color data of the previous section is an example of direct proximities. That is, the data arrives in the format of proximities. Often, this is not the case and our data does not consist of proximities between variables. However, by considering an appropriate measure, proximities can be derived from the original data. For example, consider the case where objects are rated on several variables. If the interest lies in representing the variables, we can calculate the correlation matrix as measure of similarity between the variables. MDS can be applied to describe the relationship between the variables on the basis of the derived proximities. Alternatively, if interest lies in the objects, Euclidean distances can be computed between the objects using the variables as dimensions. In this case, we use high dimensional Euclidean distances as dissimilarities and we can use MDS to reconstruct these distances in a low dimensional space.

Co-occurrence data are another source for obtaining dissimilarities. For such data, a respondent groups the objects into partitions and an $n \times n$ incidence matrix is derived where a one indicates that a pair of objects is in the same group and a zero indicates that they are in different groups. By considering the frequencies of objects being in the same or different groups and by applying special measures (such as the so-called Jaccard similarity measure), we obtain proximities. For a detailed discussion of various (dis)similarity measures, we refer to Gower and Legendre (1986).

3   Formalizing Multidimensional Scaling

To formalize MDS, we need some notation. Let n be the number of different objects and let the dissimilarity for objects i and j be given by δ_{ij}. The coordinates are gathered in an $n \times p$ matrix $\mathbf{X}$, where p is the dimensionality of the solution to be specified in advance by the user. Thus, row i from $\mathbf{X}$ gives the coordinates for object i. Let $d_{ij}(\mathbf{X})$ be the Euclidean distance between rows i and j of $\mathbf{X}$ defined as

$$d_{ij}(\mathbf{X}) = \left(\sum_{s=1}^{p} (x_{is} - x_{js})^2 \right)^{1/2}, \tag{1}$$

that is, the length of the shortest line connecting points i and j. The objective of MDS is to find a matrix $\mathbf{X}$ such that $d_{ij}(\mathbf{X})$ matches δ_{ij} as closely as possible. This objective can be formulated in a variety of ways but here we use the definition of raw-Stress $\sigma^2(\mathbf{X})$, that is,

$$\sigma^2(\mathbf{X}) = \sum_{i=2}^{n} \sum_{j=1}^{i-1} w_{ij} (\delta_{ij} - d_{ij}(\mathbf{X}))^2 \tag{2}$$

by Kruskal (Kruskal, 1964a, 1964b) who was the first one to propose a formal measure for doing MDS. This measure is also referred to as the least-squares MDS model. Note that due to the symmetry of the dissimilarities and the distances, the summation only involves the pairs ij where $i > j$. Here, w_{ij} is a user defined weight that must be nonnegative. For example, many MDS programs implicitly choose $w_{ij} = 0$ for dissimilarities that are missing.

The minimization of $\sigma^2(\mathbf{X})$ is a rather complex problem that cannot be solved in closed-form. Therefore, MDS programs use iterative numerical algorithms to find a matrix $\mathbf{X}$ for which $\sigma^2(\mathbf{X})$ is a minimum. One of the best algorithms available is the SMACOF algorithm (De Leeuw, 1977, 1988; De Leeuw & Heiser, 1980; Borg & Groenen, 1997) based on iterative majorization. The SMACOF algorithm has been implemented in the SPSS procedure Proxscal (Meulman, Heiser, & SPSS, 1999). In Section 7, we give a brief illustration of the SMACOF algorithm.

Because Euclidean distances do not change under rotation, translation, and reflection, these operations may be freely applied to MDS solution without affecting the raw-Stress. Many MDS programs use this indeterminacy to center

the coordinates so that they sum to zero dimension wise. The freedom of rotation is often exploited to put the solution in so-called principal axis orientation. That is, the axis are rotated in such a way that the variance of $\mathbf{X}$ is maximal along the first dimension, the second dimension is uncorrelated to the first and has again maximal variance, and so on.

Here, we have discussed the Stress measure for MDS. However, there are several other measures for doing MDS. In Section 8, we briefly discuss other popular definitions of Stress.

4   Transformations of the Data

So far, we have assumed that the dissimilarities are known. However, this is often not the case. Consider for example the situation in which the objects have been ranked. That is, the dissimilarities between the objects are not known, but their order is known. In such a case, we would like to assign numerical values to the proximities in such a way that these values exhibit the same rank order as the data. These numerical values are usually called disparities, d-hats, or pseudo distances, and they are denoted by $\widehat{d}$. The task of MDS now becomes to simultaneously obtain disparities and coordinates in such a way that the coordinates represent the disparities (and thus the original rank order of the data) as well as possible. This objective can be captured in minimizing a slight adaptation of raw Stress, that is,

$$\sigma^2(\widehat{\mathbf{d}}, \mathbf{X}) = \sum_{i=2}^{n} \sum_{j=1}^{i-1} w_{ij}(\widehat{d}_{ij} - d_{ij}(\mathbf{X}))^2, \tag{3}$$

over both the $\widehat{\mathbf{d}}$ and $\mathbf{X}$, where $\widehat{\mathbf{d}}$ is the vector containing $\widehat{d}_{ij}$ for all pairs. The process of finding the disparities is called optimal scaling and was first introduced by Kruskal (Kruskal, 1964a, 1964b). Optimal scaling aims to find a transformation of the data that fits as well as possible the distances in the MDS solution. To avoid the trivial optimal scaling solution $\mathbf{X} = \mathbf{0}$ and $\widehat{d}_{ij} = 0$ for all ij, we impose a length constraint on the disparities in such a way that the sum of squared d-hat's equals a fixed constant. For example, $\sum_{i=2}^{n} \sum_{j=1}^{i-1} w_{ij}\widehat{d}_{ij}^2 = n(n-1)/2$ (De Leeuw, 1977).

Transformations of the data are often used in MDS. Figure 2 shows a few examples of transformation plots for the color example. Let us look at some special cases.

Suppose that we choose $\widehat{d}_{ij} = \delta_{ij}$ for all ij. Then, minimizing (3) without the length constraint is exactly the same as minimizing (2). Minimizing (3) *with* the length constraint only changes $\widehat{d}_{ij} = a\delta_{ij}$, where a is a scalar chosen in such a way that the length constraint is satisfied. This transformation is called a ratio transformation (Figure 2a). Note that, in this case, the relative differences of $a\delta_{ij}$ are the same as those for δ_{ij}. Hence, the relative differences of the $d_{ij}(\mathbf{X})$ in (2) and (3) are also the same. Ratio MDS can be seen as the most restrictive transformation in MDS.
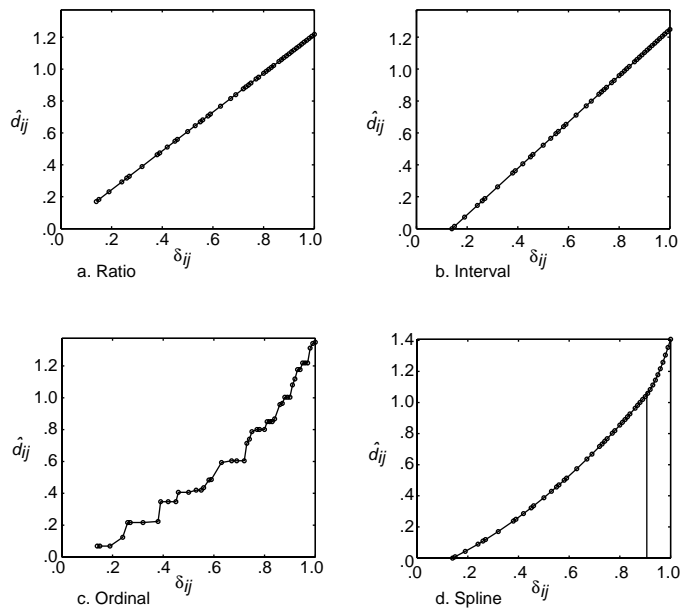
Figure 2: Four transformations often used in MDS.

An obvious extension to the ratio transformation is obtained by allowing the $\widehat{d}_{ij}$ to be a linear transformation of the δ_{ij}. That is, $\widehat{d}_{ij} = a + b\delta_{ij}$, for some unknown values of a and b. Figure 2b depicts an interval transformation. This transformation may be chosen if there is reason to believe that $\delta_{ij} = 0$ does not have any particular interpretation. An interval transformation that is almost horizontal reveals little about the data as different dissimilarities are transformed to similar disparities. In such a case, the constant term will dominate the $\widehat{d}_{ij}$'s. On the other hand, a good interval transformation is obtained if the line is not horizontal and the constant term is reasonably small with respect to the rest.

For ordinal MDS, the $\widehat{d}_{ij}$ are only required to have the same rank order as δ_{ij}. That is, if for two pairs of objects ij and kl we have $\delta_{ij} \leq \delta_{kl}$ then the corresponding disparities must satisfy $\widehat{d}_{ij} \leq \widehat{d}_{kl}$. An example of an ordinal transformation in MDS is given in Figure 2c. Typically, an ordinal transformation shows a step function. Similar to the case for interval transformations, it is not a good sign if the transformation plot shows a horizontal line. Moreover, if the transformation plot only exhibits a few steps, ordinal MDS does not use finer information available in the data. Ordinal MDS is particularly suited if the original data are rank orders. To compute an ordinal transformation a method called **monotone regression** can be used.

A monotone spline transformation offers more freedom than an interval transformation, but never more than an ordinal transformation. The advantage of a spline transformation over an ordinal transformation is that it will

yield a smooth transformation. Figure 2d shows an example of a spline transformation. A spline transformation is built on two ideas. First, the range of the δ_{ij}'s can be subdivided into connected intervals. Then, for each interval, the data are transformed using a polynomial of a specified degree. For example, a second-degree polynomial imposes that $\widehat{d}_{ij} = a\delta_{ij}^2 + b\delta_{ij} + c$. The special feature of a spline is that at the connections of the intervals, the so-called interior knots, the two polynomials connect smoothly. The spline transformation in Figure 2d was obtained by choosing one interior knot at .90 and by using second-degree polynomials. For MDS it is important that the transformation is monotone increasing. This requirement is automatically satisfied for monotone splines or I-Splines (see, Ramsay, 1988; Borg & Groenen, 1997). For choosing a transformation in MDS it suffices to know that a spline transformation is smooth and nonlinear. The amount of nonlinearity is governed by the number of interior knots specified. Unless the number of dissimilarities is very large, a few interior knots for a second-degree spline usually works well.

There are several reasons to use transformations in MDS. One reason concerns the fit of the data in low dimensionality. By choosing a transformation that is less restrictive than the ratio transformation a better fit may be obtained. Alternatively, there may exist theoretical reasons why a transformation of the dissimilarities is desired. Ordered from most to least restrictive transformation, we start with ratio, then interval, spline, and ordinal.

If the data are dissimilarities, then it is necessary that a transformation is monotone increasing (as in Figure 2) so that pairs with higher dissimilarities are indeed modelled by larger distances. Conversely, if the data are similarities, then the transformation should be monotone decreasing so that more similar pairs are modelled by smaller distances. A ratio transformation is not possible for similarities. The reason is that the $\widehat{d}_{ij}$'s must be nonnegative. This implies that the transformation must include an intercept.

In the MDS literature, one often encounters the terms metric and nonmetric MDS. Metric MDS refers to the ratio and interval transformations, whereas all other transformations such as ordinal and spline transformations are covered by the term nonmetric MDS. We believe, however, that it is better to refer directly to the type of transformation that is used.

There exist other a-priori transformations of the data that are not optimal in the sense described above. That is transformations that are not obtained by minimizing (3). The advantage of optimal transformations is that the exact form of the transformation is unknown and determined optimally together with the MDS configuration.

5   Diagnostics

In order to assess the quality of the MDS solution we can study the differences between the MDS solution and the data. One convenient way to do this is by inspecting the so-called **Shepard diagram**.

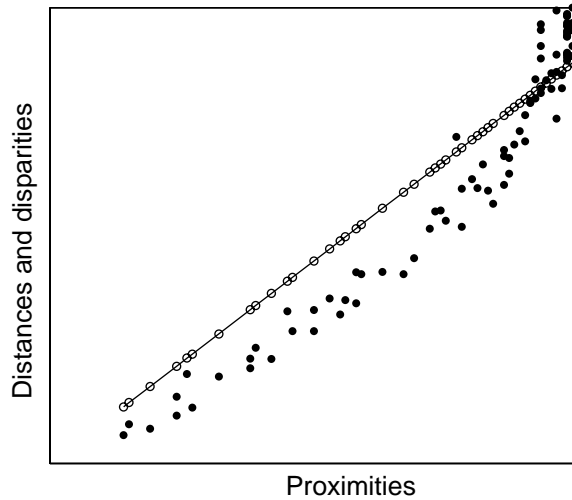A **Shepard diagram** shows both the transformation and the error. Let

Figure 3: Shepard diagram for ordinal MDS of the color data, where the proximities are dissimilarities.

p_{ij} denotes the proximity between objects i and j. Then, a **Shepard diagram** plots simultaneously the pairs $(p_{ij}, d_{ij}(\mathbf{X}))$ and $(p_{ij}, \widehat{d}_{ij})$. In Figure 3, solid points denote the pairs $(p_{ij}, d_{ij}(\mathbf{X}))$ and open circles represent the pairs $(p_{ij}, \widehat{d}_{ij})$. By connecting the open circles a line is obtained representing the relationship between the proximities and the disparities which is equivalent to the transformation plots in Figure 2. The vertical distances between the open and closed circles are equal to $\widehat{d}_{ij} - d_{ij}(\mathbf{X})$, that is, they give the errors of representation for each pair of objects. Hence, the **Shepard diagram** can be used to inspect both the residuals of the MDS solution and the transformation. Outliers can be detected as well as possible systematic deviations. Figure 3 gives the **Shepard diagram** for the ratio MDS solution of Figure 1 using the color data. We see that all the errors corresponding to low proximities are positive whereas the errors for the higher proximities are all negative. This kind of heteroscedasticity suggests the use of a more liberal transformation. Figure 4 gives the **Shepard diagram** for an ordinal transformation. As the solid points are closer to the line connecting the open circles, we may indeed conclude that the heteroscedasticity has gone and that the fit has become better.

6   Choosing the Dimensionality

Several methods have been proposed to choose the dimensionality of the MDS solution. However, no definite strategy is present. **Unidimensional scaling**, that is, $p = 1$ (with ratio transformation) has to be treated with special care because the usual MDS algorithms will end up in local minima that can be far
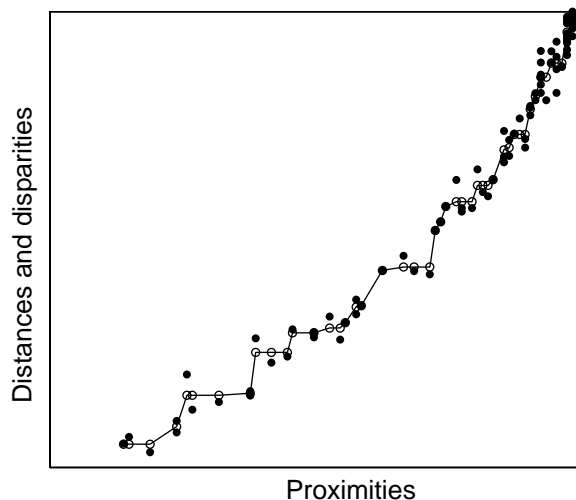
Figure 4: Shepard diagram for ordinal MDS of the color data, where the proximities are dissimilarities.

from global minima.

One approach to determine the dimensionality is to compute MDS solutions for a range of dimensions, say from 2 to 6 dimensions, and plot the Stress against the dimension. Similar to common practice in principal component analysis, we then use the elbow criterion to determine the dimensionality. That is, we choose the number of dimensions where a bend in the curve occurs.

Another approach (for ordinal MDS), proposed by Spence and Ogilvie (1973), compares the Stress values against the Stress of generated data. However, perhaps the most important criterion for choosing the dimensionality is simply based on the interpretability of the map. Therefore, the vast majority of reported MDS solutions are done in two dimensions and occasionally in three dimensions. The interpretability criterion is a valid one especially when MDS is used for exploration of the data.

7   The SMACOF Algorithm

In Section 3, we mentioned that a popular algorithm for minimizing Stress is the SMACOF Algorithm. Its major feature is that it guarantees lower Stress values in each iteration. Here we briefly sketch how this algorithm works.

Nowadays, the acronym SMACOF stands for Scaling by Majorizing a Complex Function. To understand how it works consider Figure 5a. Suppose that we have dissimilarity data on 13 stock markets and that the two dimensional MDS solution is given by the points in the horizontal plane of Figure 5a and 5b. Now, suppose that the position of the 'nikkei' index was unknown. Then we can calculate the value of Stress as a function of the two coordinates for 'nikkei'.

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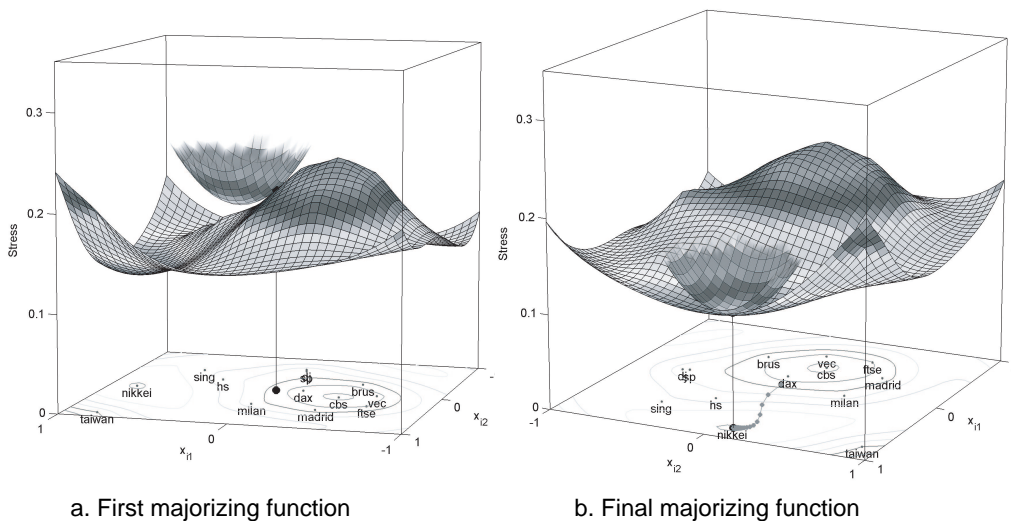a. First majorizing function   b. Final majorizing function

Figure 5: The Stress function and the majorizing function for the supporting (0,0) in Panel a., and the majorizing function at convergence in Panel b. Reproduced by permission of Vrieseborch Publishers

The surface in Figure 5a shows these values of Stress for every potential position of 'nikkei'. To minimize Stress we must find the coordinates that yield the lowest Stress. Hence, the final point must be located in the horizontal plane under the lowest value of the surface. To find this point, we use an iterative procedure that is based on majorization. First, as an initial point for 'nikkei' we choose the origin in Figure 5a. Then, a so-called majorization function is chosen in such a way that, for this initial point, its value is equal to the Stress-value, and elsewhere it lies above the Stress surface. Here, the majorizing function is chosen to be quadratic and is visualized in Figure 5a as the bowl-shaped surface above the Stress function surface. Now, as the Stress surface is always below the majorization function, the value of Stress evaluated at the point corresponding to the minimum of the majorization function, will be lower than the initial Stress value. Hence, the initial point can be updated by calculating the minimum of the majorization function which is easy because the majorizing function is quadratic. Using the updated point we repeat this process until the coordinates remain practically constant. Figure 5b shows the subsequent coordinates for 'nikkei' obtained by majorization as a line with connected dots marking the path to its final position.

8 Alternative measures for doing Multidimensional Scaling

In addition to the raw Stress measure introduced in Section 3, there exist other measures for doing Stress. Here we give a short overview of some of the most popular alternatives. First, we discuss normalized raw Stress,

$$\sigma_n^2(\widehat{\mathbf{d}}, \mathbf{X}) = \frac{\sum_{i=2}^n \sum_{j=1}^{i-1} w_{ij}(\widehat{d}_{ij} - d_{ij}(\mathbf{X}))^2}{\sum_{i=2}^n \sum_{j=1}^{i-1} w_{ij}\widehat{d}_{ij}^2}, \tag{4}$$

which is simply raw Stress divided by the sum of squared dissimilarities. The advantage of this measure over raw Stress is that its value is independent of the scale and the number of dissimilarities. Thus, multiplying the dissimilarities by a positive factor will not change (4) at a local minimum, whereas the coordinates will be the same up to the same factor.

The second measure is Kruskal's Stress-1 formula

$$\sigma_1(\widehat{\mathbf{d}}, \mathbf{X}) = \left(\frac{\sum_{i=2}^n \sum_{j=1}^{i-1} w_{ij}(\widehat{d}_{ij} - d_{ij}(\mathbf{X}))^2}{\sum_{i=2}^n \sum_{j=1}^{i-1} w_{ij}d_{ij}^2(\mathbf{X})} \right)^{1/2}, \tag{5}$$

which is equal to the square root of raw Stress divided by the sum of squared distances. This measure is of importance because many MDS programs and publications report this value. It can be proved that at a local minimum of $\sigma_n^2(\widehat{\mathbf{d}}, \mathbf{X})$, $\sigma_1(\widehat{\mathbf{d}}, \mathbf{X})$ also has a local minimum with the same configuration up to a multiplicative constant. In addition, the square root of normalized raw Stress is equal to Stress-1 (Borg & Groenen, 1997).

A third measure is Kruskal's Stress-2, which is similar to Stress-1 except that the denominator is based on the variance of the distances instead of the sum of squares. Stress-2 can be used to avoid the situation where all distances are almost equal.

A final measure that seems reasonably popular is called S-Stress (implemented in the program ALSCAL) and it measures the sum of squared error between *squared* distances and *squared* dissimilarities (Takane, Young, & De Leeuw, 1977). The disadvantage of this measure is that it tends to give solutions in which large dissimilarities are overemphasized and the small dissimilarities are not well represented.

9 Pitfalls

If missing dissimilarities are present, a special problem may occur for certain patterns of missing dissimilarities. For example, if it is possible to split the objects in two or more sets such that the between-set weights w_{ij} are all zero, we are dealing with independent MDS problems, one for each set. If this situation is not recognized, you may inadvertently interpret the missing between set distances. With only a few missing values, this situation is unlikely to happen.
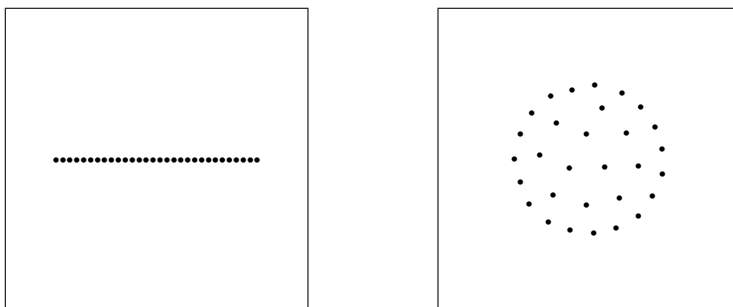
Figure 6: Solutions for constant dissimilarities with $n = 30$. The left plot shows the unidimensional solution and the right plot a 2D solution.

However, when dealing with many missing values, one should verify that the problem does not occur.

Another important issue is to understand what MDS will do if there is no information in the data, that is, when all dissimilarities are equal. Such a case can be seen as maximally uninformative and therefore as a null model. Solutions of empirical data should deviate from this null model. This situation was studied in great detail by Buja, Logan, Reeds, and Shepp (1994). It turned out that for constant dissimilarities, MDS will find in one dimension points equally spread on a line (see Figure 6). In two dimensions, the points lie on concentric circles (De Leeuw & Stoop, 1984) and in three dimensions (or higher), the points lie equally spaced on the surface of a sphere. Because all dissimilarities are equal, any permutation of these points yield an equally good fit.

This type of degeneracy can be easily recognized by checking the Shepard diagram. For example, if all disparities (or dissimilarities in ratio MDS) fall into a small interval considerably different from zero, we are dealing with the case of (almost) constant dissimilarities. For such a case, we advise redoing the MDS analysis with a more restrictive transformation, for example, using monotone splines, an interval transformation or even ratio MDS.

A final pitfall for MDS are local minima. A local minimum for Stress implies that small changes in the configuration always have a worse Stress than the local minimum solution. However, larger changes in the configuration may yield a lower Stress. A configuration with the overall lowest Stress value is called a global minimum. In general, MDS algorithms that minimize Stress cannot guarantee the retrieval of a global minimum. However, if the dimensionality is exactly $n - 1$, it is known that ratio MDS only has one minimum that is consequently global. Moreover, when $p = n - 1$ is specified, MDS often yields a solution that fits in a dimensionality lower than $n - 1$. If so, then this MDS solution is also a global minimum. A different case is that of **unidimensional scaling**. For **unidimensional scaling** with a ratio transformation, it is well known that it has many local minima and can better be solved using combinatorial methods. For low dimensionality, like $p = 2$ or $p = 3$, experiments

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indicated that the number of different local minima ranges from a few to several thousands. For an overview of issues concerning local minima in ratio MDS, we refer to Groenen and Heiser (1996) and Groenen, Heiser, and Meulman (1999).

When transformations are used, there are fewer local minima and the probability of finding a global minimum increases. As a general strategy, we advice to use multiple random starts (say 100 random starts) and retain the solution with the lowest Stress. If most random starts end in the same candidate minimum, then there probably only exist few local minima. However, if the random starts end in many different local minima, the data exhibit a serious local minimum problem. In that case, it is advisable to increase the number of random starts and retain the best solution.

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