42045. Multidimensional Scaling, Social and Behavioral Sciences (Area 4)

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Abstract: Multidimensional scaling (MDS) is a set of data-analytic tools for deriving a graphical representation of objects in a multidimensional space based on proximity relations among them (Takane, 2007). By the graphical representation, we gain intuitive understanding of the regularity governing the relationships among the objects. In this article, we introduce the basic concept and models of MDS along with its essential ingredients such as distance models, proximity data, fitting criteria, dimensionality selection. To illustrate the use of MDS, three useful MDS procedures (simple MDS, individual differences MDS, and unfolding analysis) are presented with empirical examples.

Keywords: Multidimensional Scaling, Proximity Data, Euclidean Distance Model, Individual Differences, Graphical Representation, Preference Data, Unfolding Analysis, Ideal Points.

BODY TEXT:

1. The Basic Concept of MDS

The notion of proximity (e.g., similarity/dissimilarity) among objects plays an important role in human cognition and development. It is a fundamental principle by which people categorize, generalize, and classify objects (Takane, Jung, and Oshima-Takane, 2009). Multidimensional Scaling (MDS) is a set of statistical techniques to derive a spatial map of objects based on a set of distance-like quantities among the objects. MDS represents objects as points in a multidimensional space in such a way that points corresponding to similar objects are located close together, while dissimilar objects are located far apart. The derived map from MDS facilitates our intuitive understanding of proximity relations among the objects by identifying meaningful directions or regions (object clusters) in the space.

To illustrate the use of MDS, let us take a look at similarity rating data among eight US cities presented in Table 1. The data were collected from ten university students, who were asked to indicate the degree of similarity between each pair of cities using an 11-point rating scale; a larger value indicates more similar cities. All participants completed a questionnaire with 28 pairs drawn from the eight US cities. The eight cities were: 1. Seattle, 2. New York, 3. Miami, 4. Chicago, 5. San Diego, 6. Atlanta, 7. New Orleans, and 8. Denver. PROXSCAL (Busing, Commandeur, & Heiser, 1997) implemented in SPSS (Statistical Packages for Social Sciences) was used to analyze the data, assuming that all participants have an identical object configuration. (This case is called simple MDS).

***** Insert Table 1 about here *****

Figure 1 displays the derived two-dimensional configuration of the eight US cities. The figure shows that the eight cities are roughly classified into four groups, the first group consisting of Seattle and Denver, the second consisting of Chicago and New York, the third consisting of Atlanta and New Orleans, and the fourth consisting of San Diego and Miami. Dimension 1 (the horizontal direction) contrasts New Orleans, Atlanta, New York, and Chicago with Denver, San Diego, and Seattle. We may call the horizontal direction the East-West dimension from right to left. Dimension 2 (the vertical direction), on the other hand, separates Seattle, New York, Chicago, and Denver from New Orleans, Miami, San Diego, and Atlanta. We may call the vertical direction the North-South dimension from top to bottom. It is interesting to note that participants' perception of similarity among the cities seems to be, to a large extent, determined by their geographic locations. This may be because geographic locations are a truly important factor occupying participants' mind in judging similarity among the cities, or it may be because cities located geographically close have similar climate and culture (atmosphere, people's life style, etc.).

***** Insert Figure 1 about here *****

2. Distance Models

As illustrated above, MDS represents inter-object similarities/dissimilarities by inter-point distances. The simple Euclidean distance model is most frequently used for this purpose due to its familiarity in our everyday life. This is also the model used to derive the configuration given in Figure 1. For other distance models such as the city-block distance model, see Carroll and Arabie (1998). The Euclidean distance between object points *i* and *j* (d_{ij}) is calculated by

$$d_{ij} = \left[\sum_{m=1}^{M}(x_{im} - x_{jm})^2\right]^{1/2}, \quad (1)$$

where x_{im} and x_{jm} denote the coordinates of object points *i* and *j* on dimension *m*, respectively, and *M* indicates the dimensionality (the number of dimensions) of the space. Once the coordinates of object points are obtained (through MDS), we can locate the objects in the space using a Cartesian coordinate system. Note that the Euclidean distance is invariant over the choice of origin and orientation of coordinate axes. That is, the distance does not change if the origin of the space is shifted, or the coordinate axes are rotated. It is customary to place the origin at the centroid of the object configuration, and set the coordinate axes in the principal axis directions. In principal axis directions, dimension 1 accounts for the largest possible variance among object coordinates, dimension 2 accounts for the next largest variance, given that it is orthogonal to the first dimension, and so on. The principal axis directions are not necessarily most easily interpretable, and if necessary, they may be changed to other coordinate axes having easier interpretations. The configuration displayed in Figure 1 was in fact rotated about 60 degrees clockwise from the principal axis solution provided by PROXSCAL to facilitate interpretations.

3. Proximity Data and Data Transformations

A variety of proximity data may be used in MDS, arising from a variety of data collection procedures, such as similarity ratings, sorting, same-different judgment, frequency of co-occurrences, reaction time, frequency of social interactions, and profile similarity. In similarity rating methods used to obtain the data in Table 1, objects are presented in a pair to the participants who are asked to rate the degree of similarity between them on a rating scale. In the sorting method, participants are given a set of objects and are asked to group them into several groups in terms of their similarity. The number of times two objects are put into same groups is counted over a group of participants and is used as a similarity measure between the objects. It is noteworthy that different proximity measures may reflect different aspects of proximity relations among objects, resulting in different configurations of the objects. For more systematic descriptions of the data collection methods and the related issues, see Takane et al. (2009).

Whichever data collection methods may be used, it is unlikely that observed proximity data can be directly approximated by a distance model. The data may be similarity data (as in the data given in Table 1), which are inversely related to distances. In this case, the observed similarity data must be inversely monotonically transformed in order to be fitted by a distance model. Even if the data are dissimilarity data, they may not be linearly related to underlying distances, and need to be transformed before they can be fitted by a distance model. The problem of how the observed proximity data are related to the underlying distances is generally referred to as the scale level of measurement. Different scale levels require different types of transformations of proximity data.

Four scale levels are typically distinguished in MDS: ratio, interval, log-interval, and ordinal. These distinctions are important because certain MDS procedures are only appropriate for certain scale levels. MDS procedures assuming a ratio, interval, or log-interval scale are called metric MDS, while others assuming an ordinal scale are called nonmetric MDS (Shepard, 1962; Kruskal, 1964a, b). Let o_{ijk} denote the observed proximity between objects *i* and *j* for participant *k*. In the ratio scale, proximity data are assumed approximately related to distances (d_{ij}) by $a_k o_{ijk} \approx d_{ij}$, where a_k is positive. (This is called a similarity transformation.) In the interval scaled measurement, it is assumed that $a_k o_{ijk} + b_k \approx d_{ij}$, where a_k is positive if the data are dissimilarity data, and negative if they are similarity data, and b_k is an arbitrary constant. (This is called an affine transformation.) In the log-interval scale, it is assumed that the observed proximity measures are related to underlying distances by a power transformation: $b_k o_{ijk}^{a_k} \approx d_{ij}$. If the log is taken on both sides, we obtain $a_k \ln o_{ijk} + \ln b_k \approx \ln d_{ij}$, which is a linear relationship between $\ln o_{ijk}$ and $\ln d_{ij}$, thus the name log-interval scale. In the ordinal scale level, o_{ijk} and d_{ij} are assumed to be only monotonically related. That is, $o_{ijk} > o_{i'j'k}$ implies $d_{ij} > d_{i'j'}$ if the data are dissimilarity data, whereas $o_{ijk} > o_{i'j'k}$ implies $d_{ij} < d_{i'j'}$ if the data are similarity data. In both cases, the transformation of the data can be expressed as $t_k(o_{ijk}) \approx d_{ij}$, where t_k is a monotonically increasing function if the data are dissimilarity, and it is a monotonically decreasing function if the data are similarity.

In empirical research we usually do not know exact scale levels of the observed proximity data in advance. As a practical strategy, we may start with a less strict assumption (e.g., ordinal scale), and then may switch to a stronger assumption (e.g., interval/ratio scale) if appropriate. This may help avoid applying untenable scale level assumptions to the observed proximity data.

In the example given above, the data are similarity rating data. Analysis was carried out under the assumption that the data are ordinal (an inverse monotonic transformation) with the option that tied observations may be untied after the transformation.

4. Fitting Criteria

In practical data analytic situations, an exact representation of the observed proximity data by a distance model is usually impossible due to measurement errors. MDS systematically searches for an object configuration and an optimal data transformation that minimizes the discrepancy between the transformed proximity data and the distance predictions. The discrepancy is quantified as a fit index (e.g., the normalized stress), which is also used as a fitting criterion to be minimized for estimating parameters in the model. Two broad classes of discrepancy functions have been used in MDS. One is the least squares (LS) criterion

(Kruskal, 1964a, b), and the other is the maximum likelihood criterion (Ramsay, 1977, 1982). Although the maximum likelihood criterion has some appeals for its statistical inference capabilities with data with a large sample size, the LS criterion has been far more predominantly used in MDS for its simplicity and flexibility, requiring no rigid distributional assumptions. The LS criterion is stated as

$$\emptyset = \sum_{k=1}^{K} \sum_{i<j} (t_k(o_{ijk}) - d_{ij})^2, \quad (2)$$

where t_k indicates a generic data transformation function, whose specific form depends on the scale level of proximity data, as described in the previous section. The LS MDS attempts to find the set of object coordinates x_{im} (i = 1, …, n, where n is the number of objects and m = 1, …, M), and data transformation parameters that minimize the discrepancy between the transformed proximity data ($t_k(o_{ijk})$) and predicted distances (d_{ij}). Criterion (2) usually cannot be minimized in closed form, and some sort of iterative algorithms should be used (see Borg and Groenen (2005) for more details of the optimization algorithms used in MDS). The LS criterion used in MDS may have multiple local minima, and iterative optimization procedures may converge to one of them that is not the true minimum of the criterion we wish to find. This is called the local minima problem. To circumvent this difficulty, we may obtain multiple solutions with many different initial estimates and choose the best solution among them. In all results of MDS reported in this articles, solutions were obtained with 100 random initial starts.

5. Dimensionality Selection

Dimensionality refers to the number of coordinates needed to locate objects in a multidimensional space. Two considerations should primarily be taken into account in determining the number of dimensions in MDS. First, the derived object configuration has to fit to the data at hand reasonably well. One practical strategy is to analyze the data under varied dimensionalities, say from 1 to 4, plot the fit value against the dimensionality (called a scree plot), and identify the point where the improvement in fit flattens out (called an elbow). Another important consideration is the interpretability of derived dimensions. We should retain only the meaningful dimensions that contribute to uncovering the underlying structure of proximity relations among objects.

In the example given above, the normalized raw stress values were .089 for the unidimensional solution, .034 for the two-dimensional solution, .013 for the three-dimensional solution, and .008 for the four-dimensional solution. The two-dimensional solution was considered optimal, where the improvement in fit flattened out.

5. Individual Differences MDS

As in the example given above, proximity data are typically collected from a number of participants. In the previous analysis, however, it was assumed that there were no systematic individual differences in the way the participants perceive similarities among the cities. This assumption may not be justified. There may be some interesting differences among the participants in their similarity judgments. Individual differences (ID) MDS was designed to capture both commonality and individual differences in similarity judgments (Carroll & Chang, 1970). ID MDS assumes that there is a common spatial representation of objects that applies to all individuals, while individual differences arise from differential weighting of common dimensions by different participants. It employs the weighted Euclidean distance model, which is written as

$$d_{ijk} = \left[\sum_{m=1}^{M} w_{km}(x_{im} - x_{jm})^2\right]^{1/2}, \tag{3}$$

where d_{ijk} is the distance between objects i and j for individual k, x_{im} and x_{jm} are, as before, the coordinates of objects i and j on dimension m in the common object configuration, and w_{km} is the weight attached to dimension m by individual k. The d_{ij} in (2) is replaced by d_{ijk} given above. Note that the model (3) reduces to the simple Euclidean distance model in (1) if there is no individual differences in an object configuration, i.e., w_{km} is unity for all k and m. Using the weighted Euclidean distance model, ID MDS estimates both the common object coordinates (x_{im}) and the individual differences weights (w_{km}) in such a way that the predicted distance (d_{ijk}) best matches the optimally transformed proximity data. To eliminate the scale indeterminacy between the common object configuration and the individual differences weights, the former is typically constrained to satisfy $\sum_{i=1}^{n} x_{im}^2 / n = 1$ for $m = 1, \cdots, M$, where n is the number of objects. One important characteristic of the weighted Euclidean distance model is that there is no rotational indeterminacy in contrast with the simple Euclidean model. This means that the derived dimensions have intrinsic meanings, and we should interpret them as they are.

***** Insert Figures 2 about here *****

For illustration, we applied ID MDS to the eight US Cities data discussed earlier. Again, PROXSCAL was used to analyze the similarity data, but the weighted Euclidean distance model was applied this time. The normalized raw stress also indicated that the two-dimensional solution is best (The normalized raw stress values were .089 for the unidimensional solution, .031 for the two-dimensional solution, .009 for the three-dimensional solution, .005 for the four-dimensional solution). The derived two-dimensional common configuration was very similar to the one presented in Figure 1, and thus we omitted the presentation of the common configuration obtained from ID MDS. (The only remarkable difference is in the overall size of the configuration due to the normalization constraint discussed above.) Recall that the horizontal axis (dimension 1) contrasts the East and the West, while the vertical axis (dimension 2) contrasts the North and the South. Figure 2 depicts the individual differences weights attached to the two dimensions by different individuals. Although there are overall no big individual differences in this example, three noticeable participants are identified by numbers, 1, 9, and 10. Participant 1 puts more emphasis on dimension 1 than dimension 2, whereas participant 9 puts slightly more emphasis on dimension 2 than dimension 1. Participant 1 is more sensitive to the East-West difference, while participant 9 is opposite. Participant 10 put almost equal emphasis on both dimensions. As can be seen, the weights may show interesting patterns of individual differences, which in turn may be related to participants' backgrounds (e.g., age, gender). For more examples of interesting applications of the ID MDS, see Takane (2007).

6. Unfolding Analysis

Unfolding analysis is a variant of MDS used to analyze individual differences in preference judgments (Coombs, 1964). As an example of preference data, let us look at Table 2. A group of twenty three participants were asked to rank order six different cars from the most preferred to the least preferred. The six cars used were: Honda Civic, BMW 328 Sedan, Mercedes C-Class Sedan, Lincoln Navigator, Toyota Camry, and Jeep Grand Cherokee. Tied ranks were allowed by assigning the average of ranks to them. The data are actually anti-preference data, where a smaller value indicates more preference.

***** Insert Table 2 about here *****

In unfolding analysis, each participant is assumed to have an ideal object represented as an ideal point in the same space as actual objects are represented. The distances between the ideal point and the actual object points are assumed to be inversely related to the participant's preferences on the objects; more preferred objects are located closer to the participant' ideal points, while less preferred objects are located further apart from the ideal points. Let x_{im} denote the coordinate of object i on dimension m, and y_{km} the coordinate of individual k's ideal point on dimension m. The Euclidean distance between actual object i and individual k's ideal point is calculated by

$$d_{ik} = [\sum_{m=1}^{M}(x_{im} - y_{km})^2]^{1/2}. \quad (4)$$

The coordinates of the actual objects and ideal points are determined in such a way that the preference values of the objects for particular individual are a decreasing function of the distance between them. This implies that the observed anti-preference data are interpreted as dissimilarity data between participants' ideal objects and actual objects. As a result, we obtain two coordinate matrices, one for actual object points, and the other for participants' ideal points. The two coordinate matrices are used to derive a joint plot by superposing actual objects and participants' ideal points in a joint multidimensional space.

The data in Table 2 were analyzed by PREFSCAL (Busing, Groenen, and Heiser, 2005) implemented in SPSS. An optimal solution was obtained with 100 random initial starts under the assumption of ordinal scale. The normalized stress indicated that the two-dimensional solution is optimal (The normalized stress values were .176 for the unidimensional solution, .043 for the two-dimensional solution, .004 for the three-dimensional solution). Figure 3 presents the joint MDS configuration of the participants' ideal points and the six cars. The participants are identified by the integers from 1 to 23. Note that a car is located close to participants' ideal points if it is preferred by the participants. For example, participants 4, 6, 8, and 18 are located close to Honda Civic because these participants preferred Honda Civic to any other cars, while participants 3, 5, 11, 15, and 20 are located close to BMW 328 Sedan and Mercedes C-Class Sedan, preferred to any other cars. Figure 3 also shows that the six cars are roughly classified into three groups, the first one consisting of Toyota Camry and Honda Civic, the second consisting of BMW 328 Sedan and Mercedes C-Class Sedan, and the third consisting of Lincoln Navigator and Jeep Grand Cherokee. The within-group cars have much in common, compared to the between-group cars. For example, Toyota Camry and Honda Civic are much more similar than others in that they are economic cars produced by Japanese manufacturers. As illustrated, unfolding analysis can be a very useful technique in marketing and consumer behavior research in that it allows us to understand patterns of individual differences in preference judgments on commercial products. The characteristics of individual differences in preference judgments can be further investigated by relating to product features and participants' background information. This sort of analysis may help marketing analysts to develop practical marketing strategies such as brand and product positioning. For more examples of application of unfolding analysis, refer to Takane (2007).

***** Insert Figures 3 about here *****

7. A summary and Software for MDS

MDS is a class of statistical tools to visualize the relationships among objects in a spatial map, based on proximity and/or preference measures on the objects of interest. In this article, we addressed essential ingredients of MDS, such as the distance model, proximity data, fitting criteria, and dimensionality selection. We also examined three useful models of MDS and their applications (i.e., simple MDS, individual differences MDS and unfolding analysis).

In behavioral and social science research, SPSS (Statistical Packages for Social Sciences) has predominantly been used to analyze the proximity and preference data due to its comprehensive data-analytic capabilities and user-friendly graphical interface. For ID MDS, ALSCAL (Takane, Young, & de Leeuw, 1977) implemented in SPSS has widely been used. However, PROXSCAL (Busing et al., 1997), recently implemented in SPSS, is gradually taking over the role of ALSCAL with more flexible visualizing and data-analytic features such as graphing capabilities and multiple random starts. For unfolding analysis, PREFSCAL (Busing et al., 2005), also recently incorporated in SPSS, has primarily been used in empirical research owing to its remarkable feature to overcome the degeneracy problems (e.g., all object points collapsing into one), prevalent in unfolding analysis.

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Table 1: Similarity ratings among eight US cities by ten participants (1: very dissimilar, 11: very similar). The eight US cities are: 1. Seattle, 2. New York, 3. Miami, 4. Chicago, 5. San Diego, 6. Atlanta, 7. New Orleans, and 8. Denver.

Participant	1	2	3	4	5	6	7	Participant	1	2	3	4	5	6	7
	4								9						
	6	6							2	9					
	6	9	7						10	11	9				
1	6	5	6	6				6	3	8	11	5			
	6	8	9	7	6				2	10	9	11	9		
	5	2	7	5	5	8			2	8	3	5	7	11	
	3	2	2	5	3	2	2		10	1	1	6	2	5	3
	4								5						
	2	3							1	5					
	6	7	4						3	8	4				
2	5	4	7	3				7	7	6	9	6			
	2	4	6	3	4				1	3	10	8	8		
	3	2	6	4	5	7			2	4	9	5	7	10	
	6	3	1	4	3	4	3		10	7	5	8	4	4	3
	7								7						
	5	6							4	7					
	7	10	8						8	10	6				
3	6	5	5	4				8	8	4	8	5			
	6	5	7	6	5				8	5	8	7	4		
	5	5	7	5	6	8			8	3	9	5	8	8	
	6	6	4	5	6	5	4		8	1	6	3	5	7	7
	4								8						
	3	7							5	6					
	4	10	2						8	9	5				
4	5	7	8	4				9	5	5	7	5			
	4	4	7	5	8				6	7	7	6	6		
	3	3	5	4	5	8			3	4	7	4	5	7	
	5	5	4	6	3	5	3		7	6	6	7	3	4	5
	4								6						
	1	3							5	6					
	2	9	4						9	6	3				
5	2	1	6	2				10	8	5	7	5			
	1	5	3	7	2				7	4	5	9	5		
	1	2	6	2	2	3			3	2	4	5	4	6	
	8	1	1	2	1	2	1		4	3	2	5	4	6	6

Table 2: Preference ranking among six cars by twenty three participants (1: the most preferred, 6: the least preferred). The six cars are: Honda Civic, BMW 328 Sedan, Mercedes C-Class Sedan, Lincoln Navigator, Toyota Camry, and Jeep Grand Cherokee.

Participant	Honda Civic	BMW 328 Sedan	Mercedes C-Class Sedan	Lincoln Navigator	Toyota Camry	Jeep Grand Cherokee
1	3	4	6	2	1	5
2	3	6	1	5	2	4
3	5	1	2	6	3	4
4	1	3	4	5	2	6
5	4	2	1	6	3	5
6	1	4	3	5	2	6
7	2	4	3	1	5	6
8	1	3	4	5	2	6
9	5	3	2	4	1	6
10	5	1	3	2	6	4
11	5	1	1	6	6	4
12	5	4	6	3	1	2
13	1	3	5	4	2	6
14	1	3	2	6	5	4
15	5	1	2	6	4	3
16	2	1	3	6	4	5
17	6	3	2	4	5	1
18	1	4	3	5	2	6
19	3	6	5	2	4	1
20	5	1	2	3	4	6
21	2	1	3	6	4	5
22	6	4	3	1	5	2
23	5	2	4	3	6	1

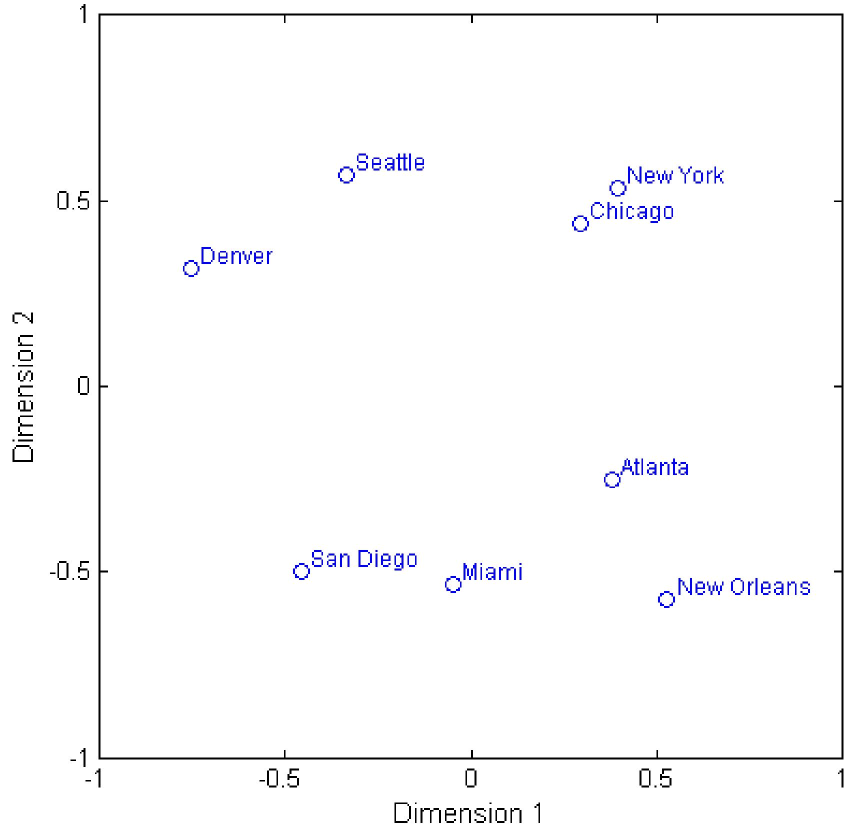

Figure 1: The two-dimensional object configuration of the eight US cities' data.

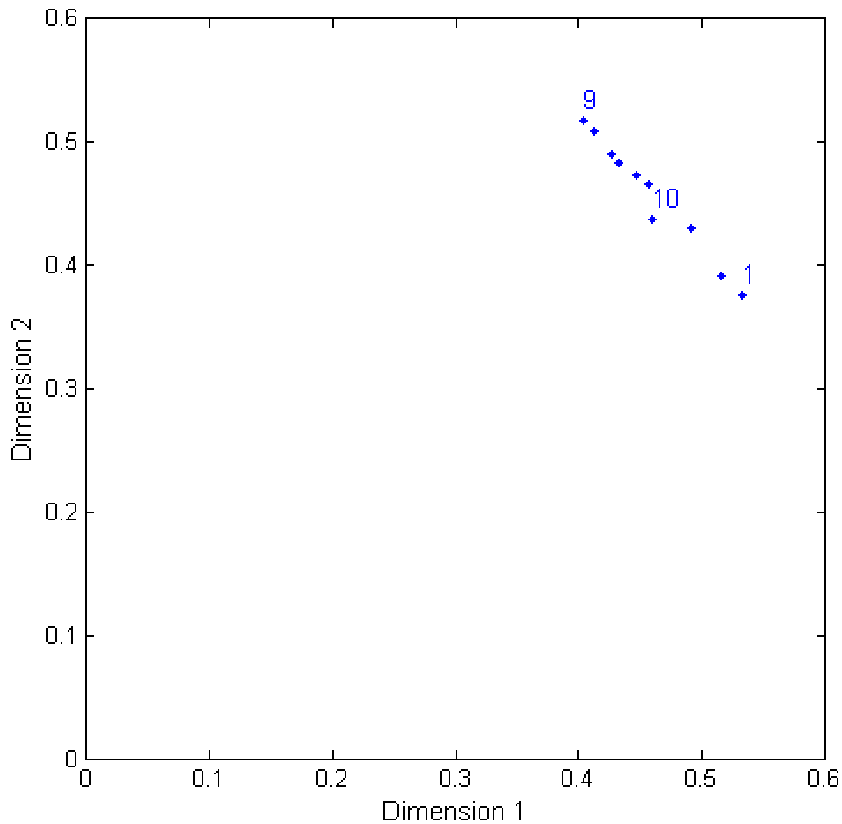

Figure 2: The plot of individual differences weights attached to the two dimensions by the ten participants.

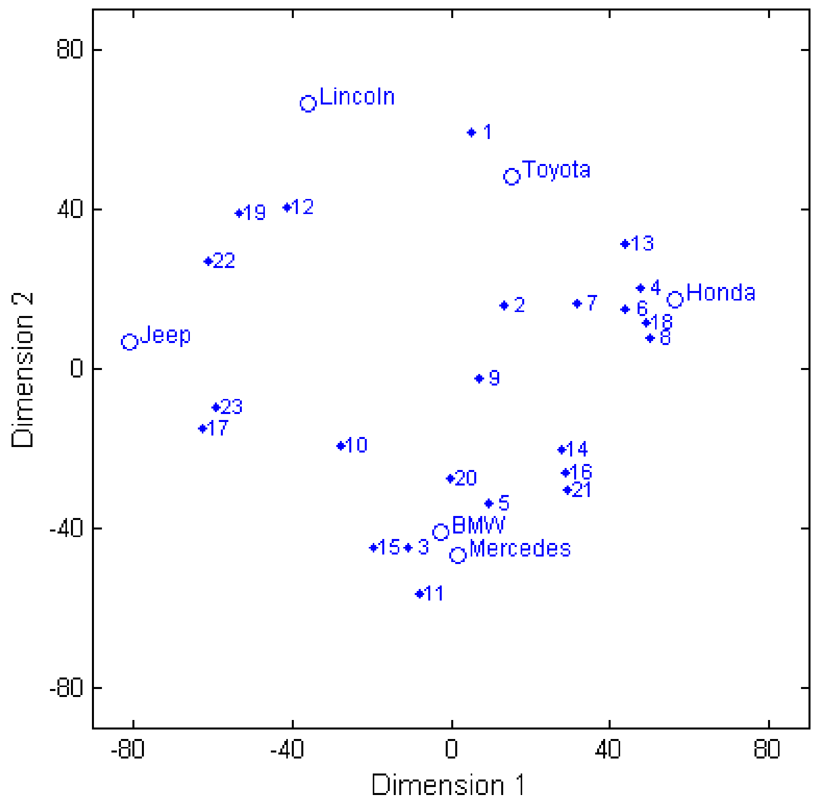

Figure 3: The joint plot of object points and participants' ideal points for the preference data on six cars. The six cars are: Honda Civic, BMW 328 Sedan, Mercedes C-Class Sedan, Lincoln Navigator, Toyota Camry, and Jeep Grand Cherokee