

Visualization of Knowledge Structures: Some Methodological Issues

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Abstract

There is a growing interest in the application of mapping techniques to gain insights into the complex structures of scientific and technological developments. Cluster analysis and projection techniques (like multidimensional scaling, principal components analysis, and self organizing maps) are essential components of the toolkits that are used for mapping of science.

Hierarchical and non-hierarchical clustering techniques (e.g. k -means) assume that boundaries between clusters (*i.e.*, domains or sub-domains of science) are sharp and do not overlap. How far is this assumption correct? Further, the projection of high-dimensional data onto low-dimensional spaces (usually two dimensional plots) inevitably leads to distortions, and greater the dimensionality of the data, greater is the distortion in the projection of individual objects. Here, a crucial question is: What is the extent of distortion and how can we assess it?

This paper responds to these concerns and illustrates the application of fuzzy cluster analysis and a technique (SPINNE) for visualization of projection distortions.

1 Introduction

Science is essentially a mosaic of fields and sub-fields. A significant feature of scientific knowledge is that cognitive boundaries of fields and sub-fields are not static; they keep on changing. Another significant feature is that these boundaries are not sharp; they tend to overlap one another.

During the past twenty five years, mapping of science has been concerned with the study of interactions and interconnections between various domains of scientific knowledge. *i.e.* its structural features. It has become an important area of research in science and technology studies (STS). Its importance can be judged from the range of its applications, which include: Identification of linkages between science and technology; Policy impact analysis; Technology opportunities analysis; Competitive intelligence; Understanding the structure and dynamics of science; Cooperation between industry and academia; etc. (*See for example:* Callon, *et al.*, 1991; Grupp, *et al.*, 1998; Korevaar and van Raan, 1992; Kostoff, *et al.*, 1998; Porter and Detampel, 1995; Zhu and Porter, 2002).

The mapping is based on the calculation and visualization of relationships between objects, such as journals, documents, authors, keywords; classification codes, etc. The methodology for science mapping is now more or less standardized. Briefly, it involves the following sequence of steps.

1. Selection of database(s).
2. Identification of objects
3. Calculation of co-occurrences of objects
4. Construction of a co-occurrence matrix and its normalization
5. Cluster analysis to group objects that are named as sub-domains. or themes
6. Visual representation of relationships between objects, using projection techniques like multidimensional scaling (MDS), principal components analysis (PCA), pathfinder networks (PFNET) and self-organizing maps (SOM).

In a recent paper, Noyons and Buter (2001) pointed out that a major problem in mapping of science is the determination of (optimal) number of clusters. There are also other problems:

1. How good is the cluster structure? Is it well defined or merely an artifact of the clustering algorithm?
2. Why should we assume *a priori* that boundaries of sub-domains of knowledge are well-demarcated and non-overlapping?

3. What about the quality of projection? In the case of MDS, a global measure of quality is ‘Stress’ (which is really a measure of badness of fit). But, what about the representation of individual objects in the map? Even when the stress is within acceptable limit, it is quite possible that some objects which are proximate in the true high-dimensional (n-D) space may not be proximate in the reduced (2-D) space, and *vice versa*. How can we visualize distortions in the projection?

This study responds to these concerns and specifically focuses on the following methodological issues: (i) What are the pros and cons of fuzzy clustering vis-à-vis crisp clustering? (ii) How do we assess the quality of cluster structure? (iii) What is the optimal number of clusters and how do we determine that? (iv) What are the distortions in the projection of high-dimensional (n-D) data onto a two-dimensional (2-D) space? These issues are discussed with reference to the mapping of cognitive structure of Mathematical Psychology, based on inter-journal citation data.

2 Methodology

The data

Inter-journal citations are deemed as an operational indicator for the disciplinary organization of science (van den Besselaar and Leydesdorff, 1996). In this study, we have attempted to map the area of Mathematical Psychology by analyzing citation relations among a set of 24 journals, which were selected on the basis of their citation links with three core journals: *J. Mathematical Psychology*, *Br. J. Mathematical and Statistical Psychology* and *Psychometrika*. The list of journals is given in Table 2. A matrix of journal-to-journal citations was constructed, which indicates the relational structure of the field along two dimensions – citing and citedness. The citing dimension reflects the active reproduction of the knowledge structure, whereas the citedness dimension reflects the codification of knowledge into the archives of scientific literature (van den Besselaar and Leydesdorff, 1996). This study is based on inter-journal citations along the citing dimension.

3 Analysis and Results

Proximity matrix

The journal-journal citation matrix was normalized and Euclidean distances among the citing journals were computed. Self citations were excluded since they do not contribute to the structure of the citation network. This resulted in a normalized symmetric matrix for subsequent cluster analysis and multidimensional scaling

Cluster analysis

Overlapping data structures can be explored through Principal Components Analysis (PCA) or fuzzy clustering algorithms. Van den Besselaar and Leydesdorff (1996) used factor analysis to classify journals in the area of *Artificial Intelligence* into different specialties. They attributed journals to specific factors on the basis of factor loadings, but some of the journals had high loadings on more than one factor, suggesting an overlapping structure. But, PCA is sensitive to outliers and poor correlations due to poorly distributed variables, and more importantly cannot deal effectively with nonlinear structures (Rassokhin *et al.*, 2001).

Prominent fuzzy clustering algorithms are: fuzzy *c*-means (Bezdek, 1981) – a fuzzification of *k*-means clustering algorithm (and its several variants) and FANNY (fuzzy analysis). In this study, we have used FANNY to group the journals into knowledge sub-domains, since it offers certain advantages over other fuzzy clustering algorithms. FANNY is based on less restrictive assumptions and more importantly yields statistics and graphical displays which help in selecting the optimum number of clusters and also in assessing the quality of cluster configuration. The algorithm is described in Kaufman and Rousseeuw (1990) and implemented in statistical software, such as WinIDAMS (UNESCO), SPLUS (Mathsoft Inc) and NCSS (Hintze, 2001).

In fuzzy clustering, each object is ‘spread over’ various clusters and the degree of belonging of an object to different clusters is quantified by means of membership coefficients (m_{ij}) which are subject to the constraint

$$0 \leq m_{ij} \leq 1 \text{ for all } i = 1, 2, \dots, n \text{ and for all } j = 1, 2, \dots, k$$

where n is the number of objects and k is the number of clusters. This is called fuzzification of the cluster configuration. It has the advantage that it does not force every object into a specific cluster and provides much more detailed information about the data structure. By convention, the sum of membership coefficients is normalized to 1.

When each object has equal membership in all clusters, the clustering is entirely fuzzy. On the other hand, when each object has a membership of 1 in some cluster and zero membership in all other clusters; the clustering is entirely crisp. The algorithm computes a coefficient, Dunn's partition coefficient $\{F(U)\}$, which indicates the extent of fuzziness of the cluster structure. This coefficient measures how close the fuzzy solution is to the corresponding crisp solution. It ranges from $1/k$ to 1.

$F(U) = 1 \Rightarrow$ Completely crisp clustering

$F(U) = 1/k \Rightarrow$ Completely fuzzy clustering

Normalized version of Dunn's coefficient, $\{Fc(U)\}$, ranges from 0 (completely fuzzy clustering) to 1 (completely crisp clustering). Kaufman and Rousseeuw (1990) have also proposed another coefficient $D(U)$. Its normalized version, $Dc(U)$ ranges from 1 (completely fuzzy clustering) to 0 (completely crisp clustering).

As mentioned earlier, two of the most difficult tasks in cluster analysis are: How to decide the appropriate number of clusters and how to distinguish a bad cluster from a good one. The algorithm computes a set of coefficients (called silhouettes) and graphical displays (silhouette plots) for the nearest crisp cluster. A silhouette measures how well an object has been classified by comparing its dissimilarity within its cluster to its dissimilarity with its nearest neighbour. It is computed as follows:

Consider an object $I \in$ Cluster A .

Let $a(I) =$ Average dissimilarity of I to all other objects in A .

Let $b(I) =$ Average dissimilarity of I to all objects in the neighbouring cluster B

$$S(I) = [b(I) - a(I)] / [\text{Max } a(I), b(I)]$$

$S (I)$ ranges between -1 and $+1$. Silhouette value close to $+1$ indicates that the object has been well classified. Silhouette value close to zero means that the object has been arbitrarily classified; in other words it lies between clusters A and B. Silhouette value close to -1 implies that the object has been misclassified. The silhouette plot shows which objects lie well within the cluster and which ones are arbitrarily or wrongly classified. A useful summary statistic is the average value of S across all objects. This summarizes how well the cluster structure fits the data. An easy way to select the appropriate number of clusters is to choose that number of clusters which maximizes the average silhouette:

The proximity matrix was submitted to the clustering algorithm for a sequence of clusters ranging from two to eight clusters, using NCSS software package. Table 1 indicates the average dissimilarity, average silhouette and coefficients indicating the fuzziness of cluster structure. It can be easily seen that a three- cluster configuration yields the maximum value of average silhouette (0.472881), maximum value of $F_c (U)$ and minimum value of $D_c (U)$ (*i.e.*, minimum fuzziness). Hence, a three- cluster solution was retained for further analysis and interpretation.

The primary output of FANNY is a list of membership coefficients (or assignment probabilities) for all the objects. Table 2 shows membership coefficients of journals in three clusters and the nearest crisp cluster. This table is self-explanatory and any elaboration would be redundant. Generally speaking, assignment probabilities of journals to the nearest crisp cluster are higher for Cluster 1 than those for Cluster 2 and Cluster 3 respectively. Looking at the titles of the journals assigned to different clusters, we can label the clusters as follows:

Cluster 1: Statistical Computation

Cluster 2: Psychological Measurement

Cluster 3: Psychology

The value of normalized Dunn's coefficient (0.2085) is much less than 1, which implies that cluster configuration is quite fuzzy. This can also be visualized from the assignment

probabilities of different journals to the nearest crisp cluster, which range between 0.3972 and 0.7560.

Table 3 shows silhouette values and silhouette plots for different journals assigned to the nearest crisp cluster. It can be easily seen that Cluster 1 is more pronounced than Cluster 2 and Cluster 3 in that order. Two journals, viz. *Psychometrika* and *Math Soc Sc*, seem to be at the outskirts of their clusters, since their silhouette values are quite low.

A series of cluster analyses ranging from 2 to 23 clusters was performed to find out if the average silhouette exceeds that obtained earlier ($S = 0.472881$). The three-cluster configuration still had the maximum average silhouette, though fuzziness decreased for very large values of k . This is understandable. For example, if 24 objects are assigned to 23 clusters, there would be hardly any scope for fuzziness. The maximum possible average silhouette is called *Silhouette Coefficient (SC)*.

According to the thumb rule suggested by Rousseeuw (1987), the Silhouette Coefficient equal to 0.472881 implies that the clustering structure is 'weak to reasonable' and should be confirmed by additional statistical methods. Hence we have supplemented cluster analysis with multidimensional scaling.

4 Multidimensional Scaling

Metric multidimensional scaling (MDS) algorithm was used to project the n-D data onto a 2-D plot. (The minimum stress value was equal to 0.19). Stress can be reduced by increasing the dimensionality of projection or by using non-metric MDS (for ordinal data), which seeks to preserve rank order of objects and not inter-object distances in the n-D space. Increasing the dimensionality of projection complicates the display and should be avoided unless the stress values are greater than the acceptable threshold (viz. 0.20). Moreover, the relationship between dissimilarities and inter-point distances in the MDS plot was found to be linear. Hence, we did not resort to non-metric MDS.

Figure 1 represents a two dimensional configuration of multivariate relations among the journals. In this figure, the journals are represented by circles of different colours to indicate

the nearest crisp cluster to which they have been assigned, and of different size to indicate the probability of their assignment. The MDS plot validates the three-cluster structure issued by FANNY.

5 Evaluation of MDS configuration

MDS algorithm is a valuable tool to visualize high-dimensional data on a two-dimensional (2-D) plane, but unfortunately, the reduction of dimensionality involves distortion. Higher the dimensionality of the data, more difficult it is to represent faithfully onto a 2-D plane. It could happen that some points which appear close to each other in the plot are not close neighbours in the high-dimensional (n-D) space, and *vice versa*. The distortions in projection may be spread over all pair-wise relationships or concentrated in just a few egregious pairs.

Projection distortions can be revealed by a computer program, SPINNE, developed by Bienfait and Gasteiger (1997). The program computes minimum spanning trees (MST) and plots them with coordinates issued by the projection algorithm. The minimum spanning trees are calculated for the original n-D space and also for the reduced 2-D space and superimposed onto the 2-D plots. If the projection is perfect, then the two plots should exactly match, but that rarely happens. The minimum spanning trees superimposed on the 2-D plots can reveal misleading close neighbours. The algorithm also computes k largest distortions in inter-point distances. Finally, the algorithm produces a coloured scale by means of which we can visualize the extent of distance distortions. Figures 2 and 3 represent the MDS plots superimposed by the minimum spanning tree computed for the n-D and 2-D spaces respectively,

The most visible distortion revealed by Fig.2 is the crossing of lines. The line connecting points 2 (*Perc Mot Sk*) and 22 (*Psychol Rev*) crosses two lines 16 (*J. Math Psy*) – 4 (*Ann Rev Psy*) and 16 (*J Math Psy*)–21 (*Psychol B*). The crossing of lines violates a fundamental assumption of the minimum spanning tree.

Other distortions can be discerned by comparing the MDS plots superimposed by MST calculated for the n-D space and that for the 2-D space. Here are instances of points connected by the shortest path in the n-D space, but not connected in the 2-D space, which means inter-point distances between respective pairs of points are greater in the 2-D space

compared to those in the n-D space. This means that citation links among the following pairs of journals are stronger than those depicted by the inter-point distances in the MDS plot.

5 (Ann Stat) –12 (JASA)
17 (JRSS) –10 (Com Stat)
1 (Psychometrika) – 13 (Com Stat)
19 (MBR) – 21(Psychol B)

The following pairs of points are connected in the 2-D space, but not in the n-D space, which means that they are situated closer in the 2-D space than in the n-D space. This means that citation links among the following pairs of journals are weaker than those depicted by the inter-pint distances in the MDS plot.

5 (Ann Stat) –17 (JRSS)
15 (J Edu Stat) –19 (MBR)
9 (Br J Math Stat Psy) – 19(MBR)
21(Psychol B) – 4 (Ann Rev Psychol)
22 (Psychol Rev) – 4 (Ann Rev Psy)
22 (Psychol Rev) – 21 (Psychol B)
22 (Psychol Rev) – 20 (Perc Psychophy)
2 (Perc Mot Sk) – 19 (MBR)

There are more distortions in projection in the left region of the two - dimensional plot: Pints19 (*MBR*), 21 (*Psychol B*) and 22. (*Psychol Rev*) seem to be the main trouble spots.

Finally, five largest distortions in inter-point distances were computed, which reveal that the distances of *Math Soc Sc* from *Ann Stat*, *Biometrics*, *Biometrika*, *JASA* and *JRSS* are maximally distorted.

Small distortions do not have much impact, and can be ignored, but particularly large distortions can threaten the cluster configuration. Again, intra-cluster distortions are less serious than inter-cluster distortions. Consider the point representing *Math Soc Sc*, belonging to Cluster 3. It has very large distance distortions from several journals belonging to Cluster 1. This implies that *Math Soc Sc* is quite misplaced in the two-dimensional plot. If this journal is shifted eastward., not only its distance distortions from *Ann Stat*, *Biometrics*, *Biometrika*, *JASA* and *JRSS* would decrease, but also the crossing of lines in the left region

of the MDS map would disappear. It may be recalled that *Math Soc Sc* was assigned to Cluster 3 with very low probability (0.3972). Silhouette value for this journal is also quite low (0.0975), suggesting that this journal could as well be assigned to its nearest neighbour (Cluster 2).

6 Concluding remarks

Cluster analysis and projection techniques like PCA, MDS and self organizing maps are essential components of the toolkits commonly used for mapping of science. Hierarchical and non-hierarchical clustering techniques are based on the assumption that clusters have sharp boundaries. This assumption is rather restrictive when we take into account interactions between and intermingling of various domains and sub-domains of science. In this respect, fuzzy cluster analysis has potential advantages over other techniques, but its interpretation is not straightforward.

Choosing the optimal number of clusters and the quality of cluster structure are other issues, which have largely been ignored in the mapping of science. The algorithm used for fuzzy clustering (FANNY) offers the possibility of addressing these issues.

Experience has shown that substantive results of fuzzy clustering algorithm (FANNY) and crisp clustering algorithm, such as PAM (Partition Around Medoids), are generally the same. (Nagpaul, 2001). In the present case, PAM and FANNY issued the same cluster structure. Compared to crisp clustering, fuzzy clustering provides important insights into the cluster configuration. It indicates the extent of fuzziness of the cluster structure, and also identifies the journals (or other bibliometric entities) that may be arbitrarily or wrongly assigned to their nearest crisp cluster. Further, one can assess whether the fuzziness of a knowledge domain has increased or decreased over a certain time-span and detect changes in assignment probabilities of different bibliometric entities to their nearest crisp cluster.

Projection techniques tend to preserve as faithfully as possible the original structure of the high-dimensional data, but some distortions are inevitable, which may result in potentially misleading plots. In this paper, an attempt has been made to assess distortions in projection and their implications for mapping of knowledge structures.

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Table 1 Summary of Fuzzy Cluster Analysis

NUMBER OF CLUSTERS DC (U)	AVERAGE DISTANCE	AVERAGE SILHOUETTE	F (U)	FC (U)	D (U)	
2	2.514281	0.386041	0.5811	0.1622	0.2132	0.4264
3	1.612188	0.472881	0.4723	0.2085	0.2389	0.3584
4	1.205258	0.311289	0.3543	0.1391	0.4087	0.5449
5	0.972188	0.259175	0.2774	0.0967	0.5477	0.6847
6	0.806085	0.189297	0.2374	0.0849	0.6142	0.7371
7	0.692300	0.199846	0.2489	0.1238	0.5665	0.6610
8	0.601054	-0.958333	0.2516	0.1446	0.5519	0.6307

Table 2 Membership coefficients of journals for different clusters

JOURNAL	NEAREST CRISP CLUSTER	PROBABILITY OF		
		CLUS 1	CLUS 2	CLUS 3
1 Psychometrika	2	0.2612	0.5367	0.2020
2 Perc Mot Sk	3	0.1405	0.2413	0.6182
3 App Psy Meas	2	0.1557	0.6221	0.2222
4 Ann Rev Psy	3	0.1291	0.2148	0.6560
5 Ann Stat	1	0.6960	0.1676	0.1364
6 App Stat	1	0.7560	0.1371	0.1069
7 Biometrics	1	0.6981	0.1674	0.1344
8 Biometrika	1	0.7550	0.1349	0.1101
9 Br J Math Stat Psy	2	0.1469	0.6686	0.1845
10 Com Stat	1	0.7015	0.1694	0.1291
11 Edu Psy Meas	2	0.1803	0.5251	0.2946
12 JASA	1	0.7063	0.1602	0.1335
13 J Class	2	0.2054	0.5673	0.2273
14 J Edu Meas	2	0.2012	0.5229	0.2760
15 J Edu Stat	2	0.2201	0.5659	0.2140
16 J Math Psy	3	0.1342	0.2045	0.6613
17 JRSS (B)	1	0.7538	0.1368	0.1094
18 Math Soc Sc	3	0.2544	0.3483	0.3972
19 MBR	2	0.1402	0.5539	0.3059
20 Perc Psychophy	3	0.1617	0.2299	0.6084
21 Psychol B	3	0.1258	0.1979	0.6763
22 Psychol Rev	3	0.1442	0.2321	0.6237
23 SMR	2	0.2259	0.5066	0.2675
24 Statistica	1	0.5305	0.2809	0.1886

Table 3 Silhouette values and silhouette bars

JOURNAL SILHOUETTE BAR	NEAREST CRISP MEMBERSHIP		SILHOUETTE VALUE	
	CLUSTER	PROBABILITY		
App Stat	1	0.7560	0.6875	
Biometrika	1	0.7550	0.6939	
JRSS (B)	1	0.7538	0.6889	
JASA	1	0.7063	0.6530	
Com Stat	1	0.7015	0.6285	
Biometrics	1	0.6981	0.6596	
Ann Statt	1	0.6960	0.6656	
Statistica	1	0.5305	0.4059	
Br. J. Math Stat Psy	2	0.6686	0.5624	
App Psy Meas	2	0.6221	0.5414	
J. Class	2	0.5673	0.4403	
J Edu Stat	2	0.5659	0.3548	
MBR	2	0.5539	0.3751	
Psychometrika	2	0.5367	0.1640	
Edu Psy Meas	2	0.5251	0.3848	
J Edu Stat	2	0.5229	0.4135	
SMR	2	0.5066	0.3413	
Psycol B	3	0.6763	0.4209	
J Math Psy	3	0.6613	0.5208	
Ann Rev Psy	3	0.6560	0.4239	
Psychol Rev	3	0.6237	0.4046	
Perc Mot Sk	3	0.6182	0.3584	
Perc Psy	3	0.6084	0.4625	
Math Soc Sc	3	0.3972	0.0975	

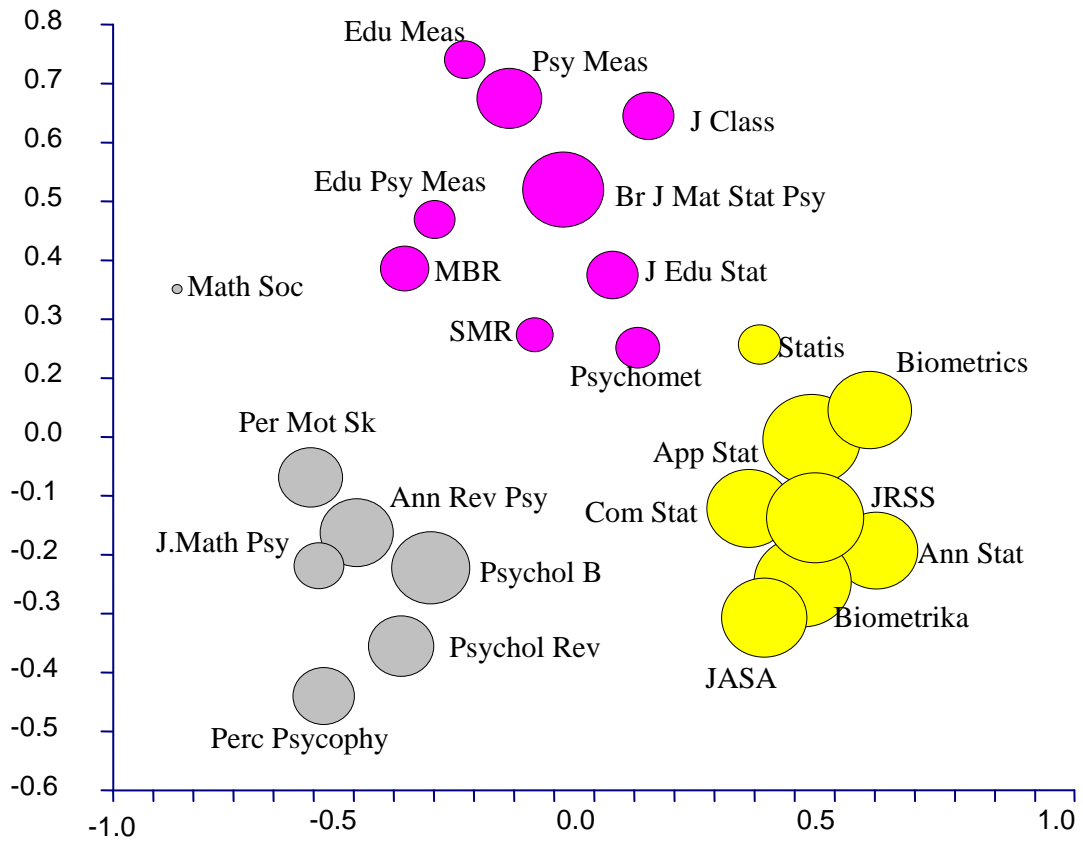


Fig. 1 MDS plot of Mathematical Psychology Journals

*Circle colour indicates the nearest crisp cluster to which the journals have been assigned.

*Circle size indicates the probability of cluster membership

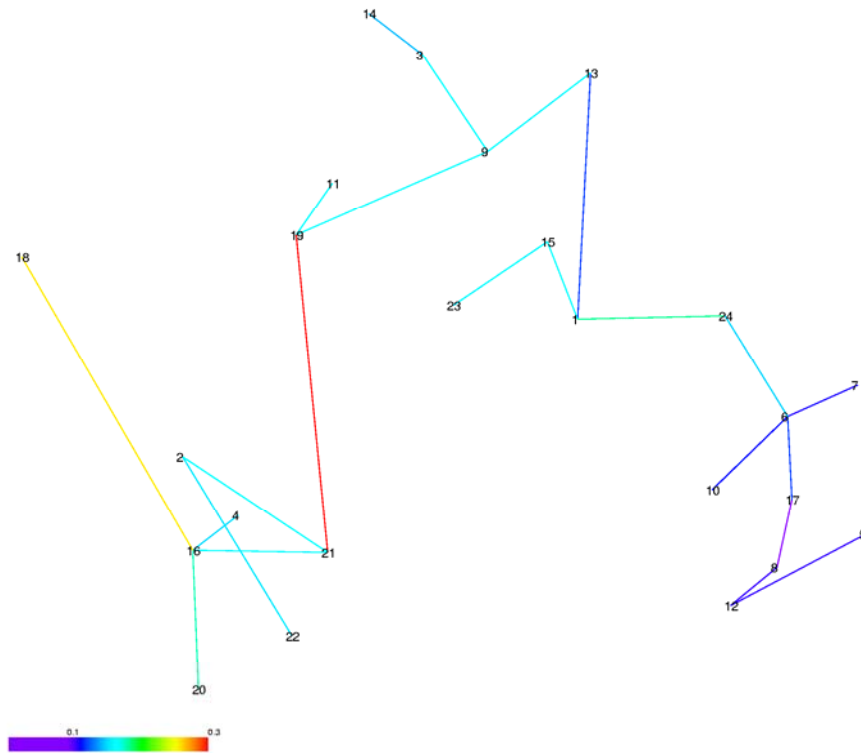


Fig. 2 Superposition of the minimum spanning tree calculated for n-D space onto the MDS plot

1 Psychometrika	9 Br J Math Stat Psy	17 JRSS (B)
2 Perc Mot Sk	10 Com Stat	18 Math Soc Sc
3 App Psy Meas	11 Edu Psy Meas	19 MBR
4 Ann Rev Psy	12 JASA	20 Perc Psychophy
5 Ann Stat	13 J Class	21 Psychol B
6 App Stat	14 J Edu Meas	22 Psychol Rev
7 Biometrics	15 J Edu Stat	23 SMR
8 Biometrika	16 J Math Psy	24 Statistica

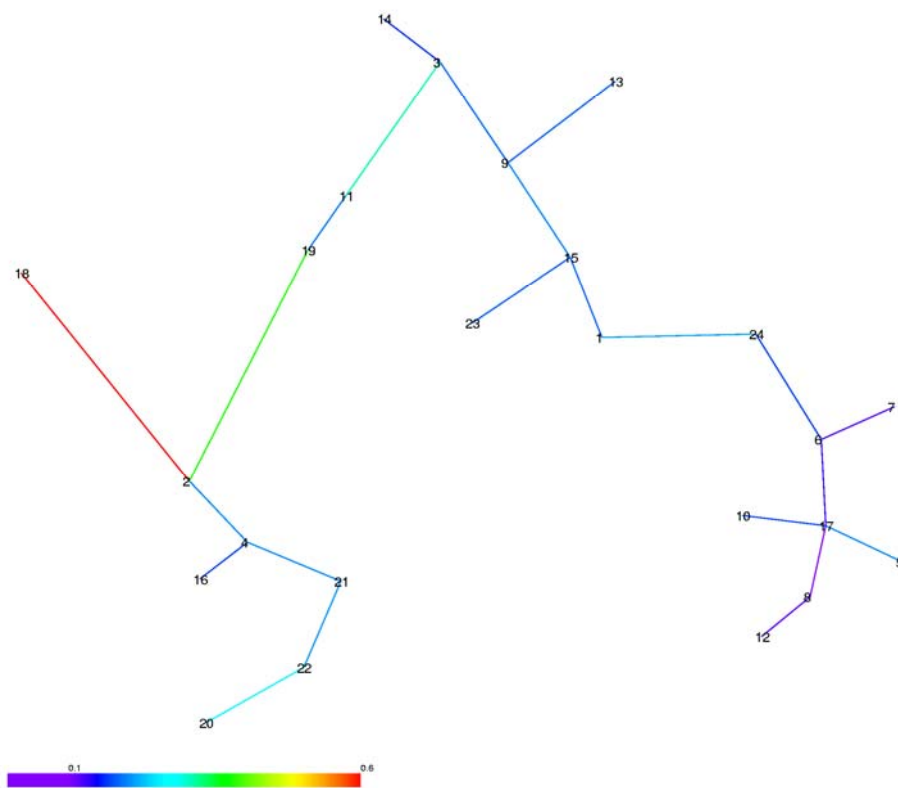


Fig. 3 Superposition of the minimum spanning tree calculated for the 2-D space onto the MDS plot

1 Psychometrika	9 Br J Math Stat Psy	17 JRSS (B)
2 Perc Mot Sk	10 Com Stat	18 Math Soc Sc
3 App Psy Meas	11 Edu Psy Meas	19 MBR
4 Ann Rev Psy	12 JASA	20 Perc Psychophy
5 Ann Stat	13 J Class	21 Psychol B
6 App Stat	14 J Edu Meas	22 Psychol Rev
7 Biometrics	15 J Edu Stat	23 SMR
8 Biometrika	16 J Math Psy	24 Statistica