VOS: A New Method for Visualizing Similarities between Objects

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VOS: A New Method for Visualizing Similarities between Objects

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Abstract

We present a new method for visualizing similarities between objects. The method is called VOS, which is an abbreviation for *visualization of similarities*. The aim of VOS is to provide a low-dimensional visualization in which objects are located in such a way that the distance between any pair of objects reflects their similarity as accurately as possible. Because the standard approach to visualizing similarities between objects is to apply multidimensional scaling, we pay special attention to the relationship between VOS and multidimensional scaling.

Keywords

Visualization of similarities, VOS, multidimensional scaling, Sammon mapping, horseshoe effect.

1 Introduction

In this report, a new method for visualizing similarities between objects is presented. The method is called VOS, which is an abbreviation for *visualization of similarities*. The aim of VOS is to provide a low-dimensional visualization in which objects are located in such a way that the distance between any pair of objects reflects their similarity as accurately as possible. Objects that have a high similarity should be located close to each other, whereas objects that have a low similarity should be located far away from each other. Because the standard approach to visualizing similarities between objects is to apply multidimensional scaling (MDS) [1], the relationship between VOS and MDS is given special attention in this report.

The report is organized as follows. In Section 2, a description of VOS is provided. In Section 3, VOS and MDS are applied to a simple example data set. The results that are obtained demonstrate an interesting property of VOS. In Section 4, the relationship between VOS and MDS is analyzed theoretically. Finally, some conclusions are provided in Section 5.

2 Description of VOS

In this section, we provide a description of VOS. Let there be n objects, denoted by $1, \ldots, n$. Let there also be an $n \times n$ similarity matrix $\mathbf{S} = (s_{ij})$ satisfying $s_{ij} \geq 0$, $s_{ii} = 0$, and $s_{ij} = s_{ji}$ for all $i, j \in \{1, \ldots, n\}$. Element s_{ij} of $\mathbf{S}$ denotes the similarity between the objects i and j. It is assumed that the similarities in $\mathbf{S}$ can be regarded as measurements on a ratio scale. VOS aims to provide a low-dimensional space in which the objects $1, \ldots, n$ are located in such a way that the distance between any pair of objects i and j reflects their similarity s_{ij} as accurately as possible. Objects that have a high similarity should be located close to each other, whereas objects that have a low similarity should be located far away from each other. The $n \times m$ matrix $\mathbf{X}$, where m denotes the number of dimensions of the space that is used, contains the coordinates of the objects $1, \ldots, n$. The vector $\mathbf{x}_i = (x_{i1}, \ldots, x_{im}) \in \mathbb{R}^m$ denotes the ith row of $\mathbf{X}$ and contains the coordinates of object i. The idea of VOS is to minimize a weighted sum of the squared Euclidean distances between all pairs of objects. The higher the similarity between two objects, the higher the weight of their squared distance in the summation. To avoid solutions in which all objects are located at the same coordinates, the constraint is imposed that the sum of all distances must equal some positive constant. In mathematical notation, the objective function to be minimized in VOS is given by

$$E(\mathbf{X}; \mathbf{S}) = \sum_{i<j} s_{ij} \|\mathbf{x}_i - \mathbf{x}_j\|^2, \tag{1}$$

where $\|\cdot\|$ denotes the Euclidean norm. The minimization of the objective function is performed subject to the following constraint

$$\sum_{i<j} \|\mathbf{x}_i - \mathbf{x}_j\| = 1. \tag{2}$$

Note that the distances $\|\mathbf{x}_i - \mathbf{x}_j\|$ in the constraint are not squared.

To provide further motivation for the objective function in (1), we note that when visualizing similarities it seems natural to expect that each object i is located close to what we call its ideal coordinates, which are given by

$$c_i(\mathbf{X}, \mathbf{S}) = \frac{\sum_j s_{ij}\mathbf{x}_j}{\sum_j s_{ij}}. \tag{3}$$

In other words, each object i may be expected to be located close to a weighted average of the coordinates of all other objects, where the coordinates of objects more similar to object i are given higher weight in the calculation of the weighted average. Locating each object i exactly at its ideal coordinates $c_i(\mathbf{X}, \mathbf{S})$ is only possible by locating all objects at the same coordinates, which clearly does not result in a useful solution. Rather than locating each object exactly at its ideal coordinates, the objective function in (1) locates objects close to their ideal coordinates. This can most easily be seen as follows. Suppose that the coordinates of all objects except some object i are fixed. Minimization of the objective function in (1) then reduces to minimization of

$$E_i(\mathbf{x}_i; \mathbf{X}, \mathbf{S}) = \sum_j s_{ij}\|\mathbf{x}_i - \mathbf{x}_j\|^2. \tag{4}$$

Minimization of (4) can be performed analytically and results in the solution $\mathbf{x}_i = c_i(\mathbf{X}, \mathbf{S})$. In other words, if the coordinates of all objects except some object i are fixed, then the objective function of VOS will locate object i exactly at its ideal coordinates. Of course, objects do not have fixed coordinates, and therefore the objective function of VOS generally does not locate objects exactly at their ideal coordinates. However, the situation with fixed coordinates clearly indicates the tendency of VOS to locate objects close to their ideal coordinates.

Finally, some approaches that are closely related to VOS have to be mentioned. The idea of visualizing similarities by locating objects close to their ideal coordinates can also be found in our earlier research [6, 7]. In this research, instead of the constraint in (2) some penalty function is used to avoid solutions in which all objects are located at the same coordinates. In [2], an approach is taken that visualizes similarities between objects by solving a constrained optimization problem. The objective function in this approach is exactly the same as in VOS, but the constraints are different. The constraints in [2] have the advantage that they allow the optimization problem to be solved as an eigenvalue problem. In our experience, however, the constraints in [2] result in less satisfactory visualizations than the constraint that is used in VOS.

3 Application to a simple example data set

In this section, we consider a simple example data set of similarities between objects. The data set is also studied in [3, 4], where it is found that a so-called horseshoe effect occurs when the similarities in the data set are visualized using multidimensional scaling (MDS). In this section, we first reproduce the result obtained in [3, 4] by applying MDS to the data set. We then apply VOS to the data set and demonstrate that VOS does not produce a horseshoe effect.

The data set consists of a 51×51 similarity matrix $\mathbf{S} = (s_{ij})$ given by

$$s_{ij} = \begin{cases} 8 & \text{if } 1 \leq |i-j| \leq 3 \\ 7 & \text{if } 4 \leq |i-j| \leq 6 \\ \multicolumn{2}{c}{\dots\dots\dots\dots\dots\dots} \\ 1 & \text{if } 22 \leq |i-j| \leq 24 \\ 0 & \text{otherwise.} \end{cases} \tag{5}$$

Visualization of the similarities in $\mathbf{S}$ using MDS results in the solution shown in Figure 1. This solution was obtained using the PROXSCAL program available in SPSS. The similarities were treated as ordinal data. As can be seen in Figure 1, MDS provides a solution in which the objects lie on a curve in the form of a horseshoe. The objects lie in the expected order, that is, object 1 is followed by object 2, object 2 is followed by object 3, and so on. However, due to the horseshoe form, there is a problem with the distances between the objects. This problem is sometimes referred to as the horseshoe effect [4]. Consider, for example, the objects 1 and 51, which are the objects lying at the ends of the horseshoe. Object 1 lies closer to object 51 than to many other objects, like object 40. Based on the solution from MDS, one would therefore expect object 1 to be more similar to object 51 than to object 40. However, this expectation is incorrect, since both the similarity between the objects 1 and 51 and the similarity between the objects 1 and 40 equal 0. Moreover, both object 1 and object 40 have a positive similarity with the objects 16 to 25, whereas there are no objects with which both object 1 and object 51 have a positive similarity. Therefore, if indirect similarities via third objects are taken into account, then object 1 is more similar to object 40 than to object 51. This is exactly opposite to the impression given by the solution from MDS.

We now consider the result of visualizing the similarities s_{ij} in (5) using VOS. The solution provided by VOS is shown in Figure 2. In this solution, the objects lie almost on a straight line. They also lie in the expected order, with object 1 followed by object 2 and so on. Interestingly,

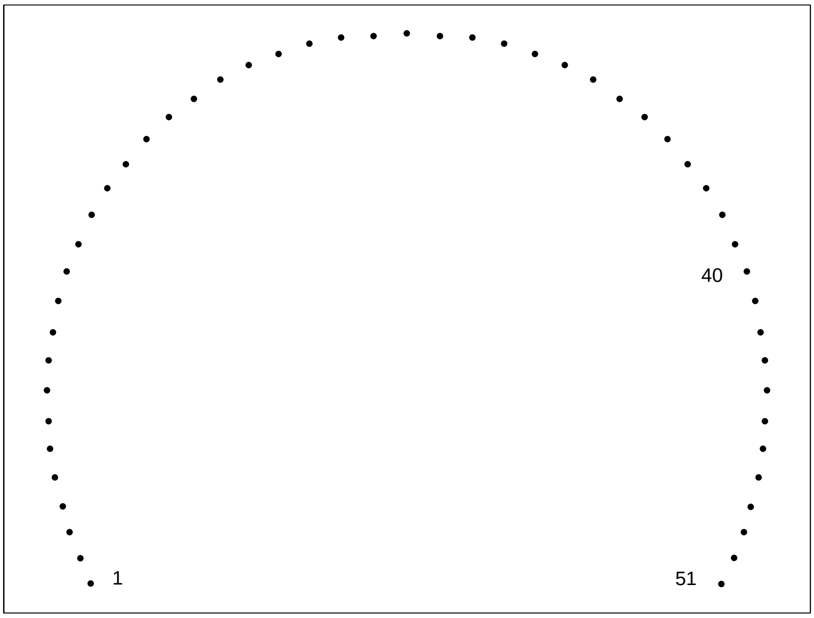

Figure 1: Visualization of the similarities s_{ij} in (5) obtained using MDS.

in contrast to the solution from MDS, the solution from VOS does not suffer from the horseshoe effect. In fact, if indirect similarities via third objects are taken into account, then the distances between the objects in the solution from VOS very accurately reflect the similarities between the objects. For example, the objects 1 and 51 lie further away from each other than the objects 1 and 40. This is exactly what one would expect based on the objects' indirect similarities. Both the objects 1 and 51 and the objects 1 and 40 have a similarity of 0, but the objects 1 and 51 do not have third objects with which they both have a positive similarity, whereas the objects 1 and 40 do have such objects, namely the objects 16 to 25. Object 1 is therefore more similar to object 40 than to object 51, and this is exactly what is reflected by the distances in the solution from VOS.

The results presented in this section indicate that VOS and MDS may provide very different solutions. In applications in which indirect similarities via third objects may contain relevant information, VOS probably provides better solutions than MDS. An example of an application where the use of VOS may be more appropriate than the use of MDS is the visualization of associations between concepts based on co-occurrence data (e.g. [6, 7]). Typically, many pairs of concepts do not co-occur at all, and these pairs of concepts then have a similarity of 0. MDS aims to provide a visualization in which for each pair of concepts with a similarity of 0 the distance between the concepts is the same. VOS seems to pay more attention to indirect

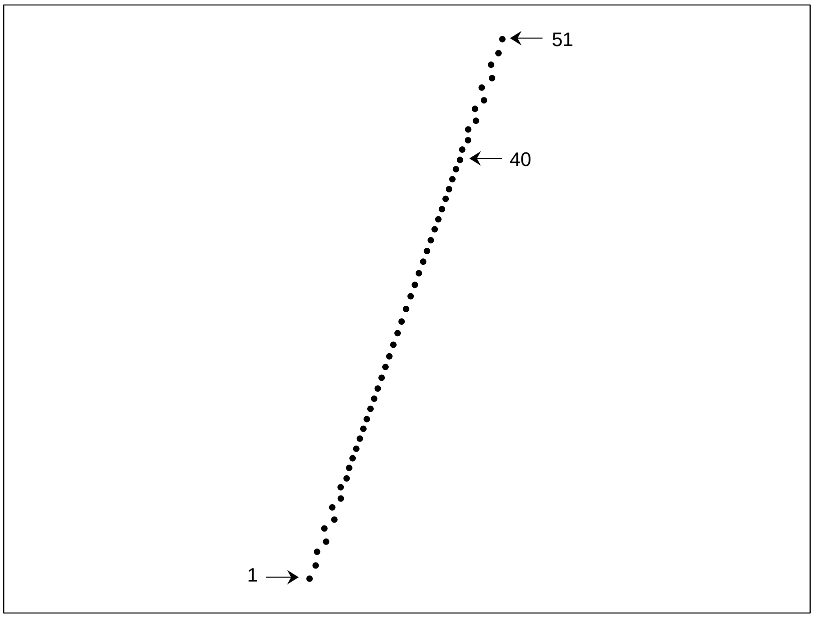

Figure 2: Visualization of the similarities s_{ij} in (5) obtained using VOS.

similarities via third concepts and may therefore locate concepts with a high indirect similarity closer to each other than concepts with a low indirect similarity. Because of this property, we expect VOS to provide more insightful visualizations of concept associations than MDS.

4 Relationship with multidimensional scaling

VOS and MDS may provide very different solutions, as we have shown in Section 3. In this section, we provide a theoretical analysis of the relationship between VOS and MDS. More specifically, we show that under certain conditions VOS is equivalent to Sammon mapping [5], which is a special variant of MDS. The mathematical notation in this section is the same as in Section 2. In addition, $\mathbf{D} = (d_{ij})$ is used to denote an $n \times n$ dissimilarity matrix satisfying $d_{ij} > 0$ and $d_{ij} = d_{ji}$ for all $i, j \in \{1, \ldots, n\}$. Element d_{ij} of $\mathbf{D}$ denotes the dissimilarity between the objects i and j. Like standard MDS, Sammon mapping aims to provide a low-dimensional space in which the objects $1, \ldots, n$ are located in such a way that the distance between any pair of objects i and j reflects their dissimilarity d_{ij} as accurately as possible. Objects that have a high dissimilarity should be located far away from each other, whereas objects that have a low dissimilarity should be located close to each other. If similarities rather than dissimilarities are available, the similarities have to be transformed into dissimilarities before Sammon mapping can be applied. We note that Sammon mapping and VOS have a very similar purpose, the difference being that Sammon mapping uses dissimilarities whereas VOS uses similarities. In Sammon mapping, the following objective function is minimized

$$\sigma(\mathbf{X};\mathbf{D}) = \sum_{i<j} \frac{(d_{ij} - \|\mathbf{x}_i - \mathbf{x}_j\|)^2}{d_{ij}}. \tag{6}$$

Sammon mapping differs from standard MDS (which is the type of MDS that is implemented in the PROXSCAL program used in Section 3) because of the division by d_{ij} in the summation in (6).

The following theorem states the equivalence, under certain conditions, of VOS and Sammon mapping.

Theorem 1 *Let $s_{ij} > 0$ for all i and j ($i \neq j$), and let similarities be transformed into dissimilarities using $d_{ij} = s_{ij}^{-1}$ ($i \neq j$). VOS and Sammon mapping are then equivalent in the sense that VOS solutions and Sammon mapping solutions differ only by a multiplicative constant.*

Proof: We start by rewriting the objective function of Sammon mapping given by (6). Substituting $d_{ij} = s_{ij}^{-1}$ in (6) gives

$$\sigma(\mathbf{X};\mathbf{S}) = \sum_{i<j} s_{ij} \left(\frac{1}{s_{ij}} - \|\mathbf{x}_i - \mathbf{x}_j\| \right)^2. \tag{7}$$

This can be rewritten as

$$\sigma(\mathbf{X};\mathbf{S}) = \sum_{i<j} \left(\frac{1}{s_{ij}} - 2\|\mathbf{x}_i - \mathbf{x}_j\| + s_{ij}\|\mathbf{x}_i - \mathbf{x}_j\|^2 \right). \tag{8}$$

The first term within the parentheses is a constant and can therefore be omitted. This results in

$$\hat{\sigma}(\mathbf{X};\mathbf{S}) = \sum_{i<j} s_{ij}\|\mathbf{x}_i - \mathbf{x}_j\|^2 - 2\sum_{i<j} \|\mathbf{x}_i - \mathbf{x}_j\|. \tag{9}$$

A VOS solution minimizes (1) subject to (2), while a Sammon mapping solution minimizes (9). To show that VOS solutions and Sammon mapping solutions differ only by a multiplicative constant, we will prove the following two statements:

(i) For each VOS solution $\mathbf{X}^{\mathrm{VOS}}$, there exists a constant c such that $c\mathbf{X}^{\mathrm{VOS}}$ is a Sammon mapping solution.

(ii) For each Sammon mapping solution $\mathbf{X}^{\mathrm{SM}}$, there exists a constant c such that $c\mathbf{X}^{\mathrm{SM}}$ is a VOS solution.

Both statements will be proven by contradiction.

We first consider statement (i). Let $\mathbf{X}^{\mathrm{VOS}}$ and $\mathbf{X}^{\mathrm{SM}}$ denote, respectively, a VOS solution and a Sammon mapping solution, and let the constant c be given by

$$c = \sum_{i<j} \left\| \mathbf{x}_i^{\mathrm{SM}} - \mathbf{x}_j^{\mathrm{SM}} \right\|. \tag{10}$$

Furthermore, define $\widehat{\mathbf{X}}^{\mathrm{SM}} = c\mathbf{X}^{\mathrm{VOS}}$ and $\widehat{\mathbf{X}}^{\mathrm{VOS}} = c^{-1}\mathbf{X}^{\mathrm{SM}}$. It follows from (10) that $\widehat{\mathbf{X}}^{\mathrm{VOS}}$ satisfies (2). Assume that $\widehat{\mathbf{X}}^{\mathrm{SM}}$ is not a Sammon mapping solution. Using (9), this assumption implies that

$$\sum_{i<j} s_{ij} \left\| \hat{\mathbf{x}}_i^{\mathrm{SM}} - \hat{\mathbf{x}}_j^{\mathrm{SM}} \right\|^2 - 2\sum_{i<j} \left\| \hat{\mathbf{x}}_i^{\mathrm{SM}} - \hat{\mathbf{x}}_j^{\mathrm{SM}} \right\| > \sum_{i<j} s_{ij} \left\| \mathbf{x}_i^{\mathrm{SM}} - \mathbf{x}_j^{\mathrm{SM}} \right\|^2 - 2\sum_{i<j} \left\| \mathbf{x}_i^{\mathrm{SM}} - \mathbf{x}_j^{\mathrm{SM}} \right\|. \tag{11}$$

In this inequality, the second term in the left-hand side equals the second term in the right-hand side. The inequality can therefore be simplified to

$$\sum_{i<j} s_{ij} \left\| \hat{\mathbf{x}}_i^{\mathrm{SM}} - \hat{\mathbf{x}}_j^{\mathrm{SM}} \right\|^2 > \sum_{i<j} s_{ij} \left\| \mathbf{x}_i^{\mathrm{SM}} - \mathbf{x}_j^{\mathrm{SM}} \right\|^2. \tag{12}$$

It then follows that

$$\sum_{i<j} s_{ij} \left\| \mathbf{x}_i^{\mathrm{VOS}} - \mathbf{x}_j^{\mathrm{VOS}} \right\|^2 > \sum_{i<j} s_{ij} \left\| \hat{\mathbf{x}}_i^{\mathrm{VOS}} - \hat{\mathbf{x}}_j^{\mathrm{VOS}} \right\|^2. \tag{13}$$

Using (1), it can be seen that this inequality implies that $\mathbf{X}^{\mathrm{VOS}}$ is not a VOS solution. However, $\mathbf{X}^{\mathrm{VOS}}$ is a VOS solution by definition. We therefore have a contradiction. Consequently, the assumption that $\widehat{\mathbf{X}}^{\mathrm{SM}}$ is not a Sammon mapping solution must be false. This proves statement (i).

We now consider statement (ii). This statement will be proven in a similar way as statement (i). Let $\mathbf{X}^{\mathrm{SM}}$ and $\mathbf{X}^{\mathrm{VOS}}$ denote, respectively, a Sammon mapping solution and a VOS solution, and let the constant c be given by

$$c = \frac{1}{\sum_{i<j} \left\| \mathbf{x}_i^{\mathrm{SM}} - \mathbf{x}_j^{\mathrm{SM}} \right\|}. \tag{14}$$

Furthermore, define $\widehat{\mathbf{X}}^{\mathrm{VOS}} = c\mathbf{X}^{\mathrm{SM}}$ and $\widehat{\mathbf{X}}^{\mathrm{SM}} = c^{-1}\mathbf{X}^{\mathrm{VOS}}$. It follows from (14) that $\widehat{\mathbf{X}}^{\mathrm{VOS}}$ satisfies (2). Assume that $\widehat{\mathbf{X}}^{\mathrm{VOS}}$ is not a VOS solution. Using (1), this assumption implies that

$$\sum_{i<j} s_{ij} \left\| \hat{\mathbf{x}}_i^{\mathrm{VOS}} - \hat{\mathbf{x}}_j^{\mathrm{VOS}} \right\|^2 > \sum_{i<j} s_{ij} \left\| \mathbf{x}_i^{\mathrm{VOS}} - \mathbf{x}_j^{\mathrm{VOS}} \right\|^2. \tag{15}$$

It then follows that

$$\sum_{i<j} s_{ij} \left\| \mathbf{x}_i^{\mathrm{SM}} - \mathbf{x}_j^{\mathrm{SM}} \right\|^2 > \sum_{i<j} s_{ij} \left\| \hat{\mathbf{x}}_i^{\mathrm{SM}} - \hat{\mathbf{x}}_j^{\mathrm{SM}} \right\|^2. \tag{16}$$

Extending both the left-hand side and the right-hand side of this inequality with an additional term, where the additional term in the left-hand side equals the additional term in the right-hand side, results in

$$\sum_{i<j} s_{ij} \left\| \mathbf{x}_i^{\mathrm{SM}} - \mathbf{x}_j^{\mathrm{SM}} \right\|^2 - 2 \sum_{i<j} \left\| \mathbf{x}_i^{\mathrm{SM}} - \mathbf{x}_j^{\mathrm{SM}} \right\| > \sum_{i<j} s_{ij} \left\| \hat{\mathbf{x}}_i^{\mathrm{SM}} - \hat{\mathbf{x}}_j^{\mathrm{SM}} \right\|^2 - 2 \sum_{i<j} \left\| \hat{\mathbf{x}}_i^{\mathrm{SM}} - \hat{\mathbf{x}}_j^{\mathrm{SM}} \right\|. \tag{17}$$

Using (9), it can be seen that this inequality implies that $\mathbf{X}^{\mathrm{SM}}$ is not a Sammon mapping solution. However, $\mathbf{X}^{\mathrm{SM}}$ is a Sammon mapping solution by definition. We therefore have a contradiction. Consequently, the assumption that $\widehat{\mathbf{X}}^{\mathrm{VOS}}$ is not a VOS solution must be false. This proves statement (ii). The proof of Theorem 1 is now complete.

We note that Sammon mapping in the way it is discussed in this section is equivalent to standard MDS where to each pair of objects i and j a weight is given that equals d_{ij}^{-1}. It therefore follows from Theorem 1 that there also exists an equivalence, under certain conditions, between VOS and the weighted variant of standard MDS.

5 Conclusions

In this report, we have presented VOS, which is a new method for visualizing similarities between objects. VOS aims to provide a low-dimensional visualization in which objects are located in such a way that the distance between any pair of objects reflects their similarity as accurately as possible. As we have discussed in this report, VOS has the following three properties. First, VOS has the tendency to locate objects close to what we have called their ideal coordinates. The ideal coordinates of an object i are defined as a weighted average of the coordinates of all other objects, where the coordinates of objects more similar to object i are given higher weight in the calculation of the weighted average. Second, VOS seems to pay more attention to indirect similarities via third objects than MDS. For example, if two objects i and j have a similarity of 0, the distance between the objects in a visualization obtained using VOS seems to depend on the number of third objects with which the objects i and j both have a positive similarity. The higher the indirect similarity via third objects, the closer the objects

i and j are located to each other. Third, although VOS and MDS may provide very different visualizations, VOS is, under certain conditions, equivalent to a special variant of MDS called Sammon mapping. Furthermore, if weights are used in MDS and these weights are chosen in the appropriate way, then there also exists an equivalence, under certain conditions, between VOS and standard MDS.

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