A New Axes Re-ordering Method in Parallel Coordinates Visualization

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***Abstract*—Visualization and interaction of multidimensional data always requires optimized solutions to integrate the display, exploration and analytical reasoning of data into one visual pipeline for human-centered data analysis and interpretation. Parallel coordinate, as one of the popular multidimensional data visualization techniques, is suffered from the visual clutter problem. Though changing the ordering of axis is a straightforward way to address it, optimizing the order of axis is a NP-complete problem. In this paper, we propose a new axes re-ordering method in parallel coordinates visualization: a similarity-based method, which is based on the combination of Nonlinear Correlation Coefficient (NCC) and Singular Value Decomposition (SVD) algorithms. By using this approach, the first remarkable axe can be selected based on mathematics theory and all axis are re-ordered in line with the degree of similarities among them. Meanwhile, we would also propose a measurement of contribution rate of each dimension to reveal the property hidden in the dataset. At last, case studies demonstrate the rationale and effectiveness of our approaches: NCC reordering method can enlarge the mean crossing angles and reduce the amount of polylines between the neighboring axes. It can reduce the computational complexity greatly in comparison with other re-ordering methods.**

Keywords-Multidimensional data visualization； visual analytics； parallel coordinates； axes re-ordering； singular value decomposition； nonlinear correlation coefficient.

I. INTRODUCTION

Multi-dimensional data analysis is becoming a commonplace as the number of applications increases, such as statistical and demographic computation, digital libraries and so on. However, traditional visualization techniques for these datasets usually require dimensionality reduction or selection to generate the meaningful visual representations. Dimensionality reduction, as Sara Johansson et.al pointed out, is always employed prior to visualization for dealing with the data with a large number of attributes[1]. Currently, many dimensionality reduction methods are able to preserve the information inside the data as much as they can by removing some less relevant data items or attributes from the original dataset. While dimension selection is mainly referred to dimension re-ordering which means that the corresponding axe of the dimension in a parallel coordinate visualization can be positioned in accordance to some effective rules such as similarity of dimensions to achieve good visual structures and patterns. This paper focuses on the dimension re-ordering rather than dimension reduction to address the problems of visual clutter and computational complexity.

In 1998, Mihael Ankerst et al. [2] presented a method which uses the similarity of dimensions to improve the quality of visualization of multidimensional data, using global and partial similarities for one or two-dimensional visualization methods. Pearson's Correlation Coefficient (PCC) is one of the most commonly used measurements for measuring similarity between two dimensions. PCC can be used for dimension reduction, clutter reduction and clustering et al. in visualization. At the same time, it has also been proved that the PCC based re-ordering problem is a NP-complete problem. Therefore, many researchers have applied heuristic algorithms to find out an optimal order of axes (or dimensions) in multi-dimensional visualization.

Though the traditional heuristic algorithms can help in finding an optimal order of axes for one- or two-dimensional visualizations, most studies have not done a deeper investigation on how to determine the first dimension (the most significant dimension) in multi-dimensional data visualizations. The first dimension always attracts much more user's attention than the others. Therefore, we may consider the one with the highest contribution rate as the first dimension to simplify the traditional similarity-based re-ordering methods and to find out the optimal order of parallel axes in a short time period.

In the paper, we firstly propose a method based on the Singular Value Decomposition (SVD) to find out the contribution of each dimension in the dataset. And then, we present a similarity-based re-ordering method in parallel coordinates which is based on the combination of a Nonlinear Correlation Coefficient (NCC) and the SVD algorithms, which is sensitive to any relationship, including the linear dependence [26]. In our experiments, we show the effectiveness of our new method by visualizing the patterns and enlarging the mean crossing angles for better visual representation. It should be noticed that the proposed method can be easily applied to the other visualization techniques.

The paper is organized as follows. Section 2 summarizes the current researches on similarity measure and dimension reordering in high-dimensional data visualization. Section 3 presents our dimension reordering approaches in detail. Section 4 describes the experimental evaluation for our new ideas, showing the effectiveness of our methods in parallel coordinates visualization. Conclusions and future work are presented in section 5.

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II. RELATED WORK

An effective way to improve the quality of multi-dimensional visualizations is to re-order the dimension axes in parallel coordinates based on similarity of data attributes. In this section, we summarises the previous research works done in the area of high-dimensional visualization.

Parallel coordinates[3, 4], scatter plot matrix[5], table lens[6] and pixel-oriented display[7] et al. are well-known and accepted visualization techniques for high-dimensional datasets. Similarity measure as one aspect of quality metrics in high-dimensional data visualization has been addressed in the past few years [1, 8-11]. It is worth noting that Enrico Bertini et al.[8] systematically presented an overview of quality metrics in many visualization techniques through a literature review of nearly 20 papers and considered correlation between two or more dimensions to be the main characteristic of similarity measure. Sara Johansson[1] introduced a weighted quality metrics to their task-dependent and user-controlled dimensionality reduction system, where small correlation values were ignored to reduce the dataset that preserved the important structures within the original dataset. Andrada Tatu et al. proposed similarity-based function for classified and unclassified data based on Hough Space transform on the resulting image of parallel coordinates [10, 11]. Aritra Dasgupta et al. [9] introduced binned data model and branch-and-bound algorithm as the screen-space metrics for parallel coordinates to reduce the computations and find the optimal order of axes.

To enhance the high-dimensional data visualization, some studies on dimension reordering have been done to find good axes layouts in visualization techniques both in one- or two-dimensional arrangement[1, 8-10, 12] [13, 14] [2, 15-18]. Mihael Ankerst et al. [2] defined similarity measures which determined the partial or global similarity of dimensions and argued that the reordering based on similarity could reduce visual clutter and do some help in visual clustering. Wei Peng et al.[15] introduced the definition of the visual clutter in parallel coordinates as the proportion of outliers against the total number of data points and they tried to use the exhaustive algorithm to find the optimal axes order for minimizing the member of edge crossings (or visual clutter). As mentioned in [16], the computational cost $O(n \cdot n!)$ hampers applications of this technique to large high dimensional data sets. Almir Olivette Artero et al. [16] introduced the dimension configuration arrangement based on similarity to alleviate clutter in visualizations of high-dimensional data. They proposed a method called SBAA (Similarity-Based Attribute Arrangement), which is a straightforward variation of the Nearest Neighbor Heuristic method, to deal with both dimension ordering and dimensionality reduction. Other studies have been done on the dimension reordering based on the similarity[11, 17, 18] [19] [20]. Michael Friendly et al.[17] designed a framework for ordering information including arrangement of variables. However, the arrangement of variables is decided mainly according to the users' desired visual effects. J. Yang et al. [18] established a hierarchical tree structure over the attributes, where the similar attributes were positioned near each other. Diansheng Guo [19] developed a hierarchical clustering method, which was based on comparison and sorting of dimensions by use of the maximum conditional entropy. Georgia Albuquerque et al. [20] introduced the quality measures to define the placement of the dimensions for Radviz and also to appraise the information content of pixel and Table Lens visualizations.

To sum up, most of the current dimension reordering methods are based on Pearson's correlation coefficient. From the statistics point of view, PCC is a method for measuring the linear correlation between the two random variables. Therefore, it is partial that we reorder the dimensions according to their similarity only depending on the calculation of PCC. Though Pargnostics, proposed by Aritra Dasgupta et al. in[1], is the most similar with our approach, the probability and joint probability during the computational process are both denoted as their special axis histograms, which lack the support by mathematical theories. Moreover, it can be seen from the definition of the mutual information that it does not range in a definite closed interval as the correlation coefficient does, which ranges in $[-1,1]$.

Hence, it is of great importance that a comprehensive and useful method should be proposed for correlation analysis among the dimensions for conveying better visual structures and patterns. In this paper, we propose similarity-based reordering method for dimensions reordering in parallel coordinates to solve the above problems.

III. METHODOLOGY

The ordering of dimensions has large impact on how easily we can perceive different structures in the data[2]. Completely different displays and conclusions may be obtained if we interactively switch between different dimension reordering. How to reorder the dimensions in high-dimensional datasets meaningfully is one of the most significant problems of the researches on quality metrics in data visualization due to its influences on the quality of visualization in terms of readability and understandability. In this section, we visualize them in a more rational way rather than arrange them only according to the empiricism.

Throughout this section the following notation is used: a dataset D is composed of n dimensions (variables) with m data items for each one. In some cases we need to measure the statistical characters between the two dimensions X and Y, where

$X = (x_1, x_2, \cdots, x_n)^T$, $Y = (y_1, y_2, \cdots, y_n)^T$.

A. Linear/Nonlinear Correlation

The correlation of two variables (dimensions/attributes) is a statistical technique that can indicate the magnitude relationship between the two variables. It also shows how the two variables interact with each other. In this section, we present the reordering methods based on the two correlation measures: Pearson's correlation and nonlinear correlation information measures.

Pearson's Correlation Coefficient [22], as one of the most popular similarity measures in visualization of multidimensional data, is a linear correlation measurement for each pair of random variables:

$$r = \frac{S_{xy}}{\sqrt{S_{xx} S_{yy}}}$$

where $S_{xx} = \sum_{i=1}^{n} (x_i - \bar{x})^2$, $S_{yy} = \sum_{i=1}^{n} (y_i - \bar{y})^2$, $S_{xy} = \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})$, $\bar{x}$ and $\bar{y}$ behave the mean of variables X and Y respectively. The value of PCC ranges in the closed interval [-1, 1], which indicates the linear correlation degree of the two variables. When the PCC value is close to 1 or -1 it denotes a strong relationship and if it close to 0 it means a weak relationship between the two variables. A positive and negative correlation coefficient denotes that both variables are in the same way or in the opposite way

Although, linear correlation can detect the relationship between two dependence variables, in the real world the correlations can also be nonlinear. Mutual Information can be thought of as a generalized correlation analogous to the linear correlation coefficient, but sensitive to any relationship, not just linear correlation. Moreover, NCC is a method that can measure nonlinear relationship based on mutual information[23, 24] and redundancy[25], which is sensitive to any relationship, not just the linear dependence[26]. Zhiyuan Shen et al.[26, 27] did further researches on the effects of statistical distribution to it and made it range in a closed interval $[0,1]$.

Corresponding to the literature[2], we mainly apply NCC to compute the partial similarity measures of dimensions in multidimensional data visualization, while SVD is used for measuring the global one. We introduce the detailed NCC in the following paragraphs. Mutual information plays an important role in the computation of NCC, which is defined as

$$I(X;Y) = H(X) + H(Y) - H(X;Y) \tag{1}$$

where $H(X)$ is the information entropy of variable X:

$$H(X) = -\sum_{i=1}^{n} p_i \ln p_i$$

$H(X;Y)$ is the joint entropy of the variables X and Y:

$$H(X;Y) = -\sum_{i=1}^{n}\sum_{j=1}^{n} p_{ij} \ln p_{ij}$$

p_i denotes the probability distribution that random variable X takes the value x_i, and p_{ij} denotes the joint probability distribution $p(X = x_i, Y = y_i)$ of the discrete random variables X and Y.

After revising joint entropy of the two variables X and Y,

$$H^r(X;Y) = -\sum_{i=1}^{b}\sum_{j=1}^{b} \frac{n_{ij}}{n} \log_b \frac{n_{ij}}{n} \tag{2}$$

in which $b \times b$ rank grids are used to place the sample pairs $\{(x_1, y_i)\}_{1 \le i \le n}$. n_{ij} is the number of samples distributed in the $ijth$ rank grid, Wang et al. [27] proposed the calculation method for nonlinear correlation coefficient as follows:

$$\begin{aligned} NCC(X;Y) &= H^r(X) + H^r(Y) - H^r(X;Y) \\ &= 2 + \sum_{i=1}^{b}\sum_{j=1}^{b} \frac{n_{ij}}{n} \log_b \frac{n_{ij}}{n} \end{aligned} \tag{3}$$

In the following section B, we apply the above formula to measure the linear or nonlinear relationship between the two dimensions in multidimensional datasets because of its sensitivity to any relationship.

B. Similarity-based Reordering

Since the problem of dimension reordering is similar to the Traveling Salesman problem, many researchers applied heuristic algorithms, such as genetic algorithms, colony optimization and nearest neighbor heuristic method etc. [2, 16], to overcome exhaustive time. In the method SBAA proposed by Almir Olivette Artero et al.[16], the largest value $s_{i,j}$ in their similarity matrix s (lower diagonal) is considered to be the initial dimension "ij" in the new order. And then, they try to search for the dimensions which will be positioned in the left and the right of it. It seems rational that we just reorder all the dimensions in line with this similarity. However, some dimensions always attract much more concentrations from the whole visual structure. For example, in parallel coordinates, the first and the last dimensions can draw much more attention than the other axes do. Therefore, different from the existed methods, we propose a new dimensions reordering algorithm based on the NCC and SVD algorithms. These methods help users reduce the computation complexity and improve the visual readability greatly.

We define the similarity matrix s, which is symmetric, as follows:

$$s = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1n} \\ s_{21} & s_{22} & \cdots & s_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ s_{n1} & s_{n2} & \cdots & s_{nn} \end{bmatrix}$$

where $s_{ij} = s_{ji}$ $(i \neq j)$, which are calculated by use of nonlinear correlation coefficient. s_{ii} $(i = 1, 2, \cdots, n)$ (We also can denote them as v_{1i}) behaves the contribution value of the ith dimension to the whole data values, which is calculated by SVD algorithm.

Similarity-based Reordering Algorithm

Step1. Form the matrix D of the data sets.

Step2. Calculate the singular value decomposition [21] of matrix D, and get the contribution factors $s_{ii}, i = 1,2,\cdots,n$.

Step3.Compute the other elements s_{ij} of similarity matrix s, using our nonlinear correlation coefficient method, besides s_{ii}, $i = 1,2,\cdots,n$ which have calculated in step2.

Step4. Choose the largest value of s_{ii}, $i = 1,2,\cdots,n$ as the extreme left attribute to start display the data sets. We denote this attribute as S_{ll}, $l \in \{1,2,\cdots,n\}$.

Step5. Get the largest value S_{ll} from $\{S_{li}, l < i\}$. Therefore, the $r_1 th$ attribute is appended to the lth attribute. We get the first two elements of neighbouring sequence $NS = \{l, r_1\}$.

Step6. Repeat step5 using the $r_1 th$ attribute as the left neighbouring attribute from $\{S_{r_1 i}, r_1 < i\}$ until inserting all attributes into the NS.

It is worth noting that this visualization method can not only provide us the similarities between each pair of dimensions, but also express some ideas of the self-property of each dimension. During the computation process of the nonlinear correlation coefficient, we chose the $b \times b$ rank grids according to the empirical formula, which is mentioned in [28]:

$$b = 1.87 \times (n-1)^{2/5} \tag{4}$$

Moreover, it is natural that we can compute the contribution rate of each dimension to the whole dataset using the following possible measure:

$$C_i = \frac{v_{1j}}{\sum_{j=1}^{n} v_{1j}} \times 100\% \tag{5}$$

This approach not only provides us a new reordering method helping us take much more insights into the dataset but also gives rise to the following new method which can help in determination of the first dimension with the most contribution.

IV. CASE STUDIES

To demonstrate the effectiveness of our rational dimension reordering methods, we analyzed many datasets in this section, Cars and Liver Disorders data set for our similarity-based reordering method. All of these data sets we tested come from the literature [29].According to the literature [30], larger crossing angle the two polylines make, the less cognitive load and the better visualization efficiency is. Therefore, to show the advantages in the readability and understandability of our method, we calculated the mean angles occurred among the polylines between two neighboring attributes using the following formula:

$$mean\_angle = \frac{total\_angle}{total\_edge\ cros\sin g}.$$

A. Cars dataset

Based on the theory in section 3, the similarity matrix of Cars data set was calculated as the following s.

$$s = \begin{bmatrix} 0.0067 & 0.5950 & 0.3236 & 0.0561 & 0.9078 & 0.8104 & 0.0302 \\ 0.5950 & 0.0018 & 0.5806 & 0.5028 & 0.8944 & 0.0261 & 0.6288 \\ 0.3236 & 0.5806 & 0.0354 & 0.1313 & 0.5223 & 0.9544 & 0.0104 \\ 0.0561 & 0.5028 & 0.1313 & 0.9991 & 0.3389 & 0.6968 & 0.0302 \\ 0.9078 & 0.8944 & 0.5223 & 0.3389 & 0.0047 & 0.9598 & 0.0197 \\ 0.8104 & 0.0261 & 0.9544 & 0.6968 & 0.9598 & 0.0235 & 0.0117 \\ 0.0302 & 0.6288 & 0.0104 & 0.0302 & 0.0197 & 0.0117 & 0.0004 \end{bmatrix}$$

After positioning the first dimension "Weight", which enjoys its significant contribution to the whole data set, we try to find out the one from the unordered dimensions with the largest similarity value to this dimension: $s_{46} = 0.6968$. Therefore, the $6-th$ dimension is considered to be the strongest correlation with the $4-th$ one. And then, we make the $6-th$ attribute to be appended to the $4-th$ one. Similar to this process, we can get the final rational dimension order, which is

$$4 \to 6 \to 5 \to 1 \to 2 \to 7 \to 3$$

Corresponding to the initial Cars dataset, the reordering dimensions calculated using our algorithm is

$$\text{Weight} \to \text{Year} \to \text{Acceleration} \to \text{MPG}$$
$$\to \text{Cylinders} \to \text{Origin} \to \text{Horsepower}$$

The reordering results after our analysis are visualized in parallel coordinates in Fig. 1(a).

We visualize Car dataset using the traditional reordering method-Pearson's Correlation Coefficient in Fig. 1(b). The corresponding order of dimensions is as follows:

$$\text{Weight} \to \text{Cylinders} \to \text{Horsepower} \to \text{MPG}$$
$$\to \text{Year} \to \text{Acceleration} \to \text{Origin}$$

Comparing with these two images in Fig. 1, we can find that visualization structures between the "Cylinders" and "Origin" dimensions with our method are clear and simple. In the visualization graph of NCC, the mean angle between the attributes "Acceleration" and "MPG" gets to 22.359°. Moreover, the mean angle between "Cylinders" and "Origin" attributes is 28.162°.Compared to the mean angle of the overall polylines produced in the PCC reordering method, 0.422°, the angle in NCC reordering one is 21.2 times larger than it. Therefore, we can find the visual effect of our reordering method is much better than the traditional one.

Table 1 presents the detailed comparisons between the similarity values of attributes, which are calculated using PCC and NCC. The numbers from 1 to 7 denote the dimensions: "MPG, Cylinders, Horsepower, Weight, Acceleration, Year and Origin" separately. Note that no matter which method we use, the similarities between the two dimensions are the same, that is $s_{ij} = s_{ji}$ $(i \neq j)$. It is obvious that there are big differences between the similarity values with two methods. For example, to our knowledge,

the similarity between the $3-th$ ("Horsepower") and $7-th$ ("Origin") dimensions of the dataset is not strong enough at all. However, the result of PCC is 0.4552, comparing to ours result 0.0104.

B. *Liver disorders dataset*

Liver Disorders dataset consists of 345 instances with 7 dimensions. Fig. 2 illustrates us the final visualization result of the whole dataset according to their similarities calculated by NCC and PCC methods respectively, where the dimension"MCV" enjoys its most significant contribution to the whole dataset and occupies the first place in the two reordering visualization.

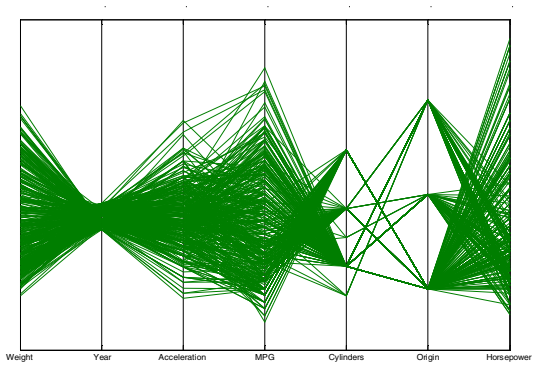
It is easy to find that the polylines among the "SF" and "DN" attributes are much less than any others among the neighboring attributes no matter in Fig. 2 (a) or (b). The mean crossing angle of these two dimensions, 43.515°, as the largest one in the dimensions reordering visualizations as well, simplifies the visual representation greatly. The mean crossing angle of our NCC reordering method to this dataset is 12.322°, which is 3.722° larger than the result calculated using PCC method.

We also tested the other datasets such as Nursery, Iris et al. large scale ones to illustrate the advantages of our methods, which all showed us that our methods can enlarge the mean crossing angles for better visualization.

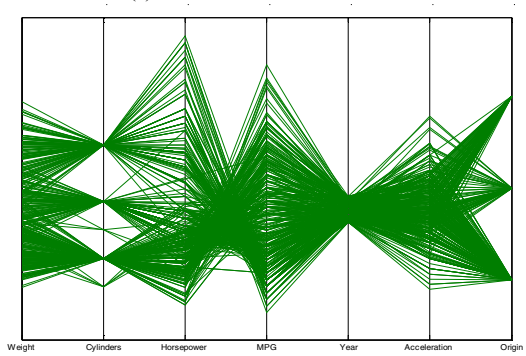
V. CONCLUSIONS AND FUTURE WORK

In this paper, we proposed a new method to improve the readability and understandability of parallel coordinates visualization theoretically. At the first stage, we propose a new way of looking into the dimensions within datasets based on the singular value decomposition algorithm. At the second stage, we present a method, named similarity-based reordering method, for calculating the similarity between the two dimensions based on the nonlinear correlation coefficient and singular value decomposition algorithms rather than the traditional Pearson's correlation coefficient, and then visualize the optimal dimension order according to the similarity in parallel coordinates. We have conducted the experimental evaluations to demonstrate the effectiveness and rationale of our approaches: NCC reordering method enlarges the mean crossing angles of the whole data set and reduces the amount of polylines between some neighboring dimensions.

During the process of calculation for nonlinear correlation coefficient, the more exact choice of rank grids will do much more help in the speed of calculation. Therefore, we consider this problem to be our first future work. And then we will apply our methods with interactive techniques to more real-world datasets and help users analyze the datasets using visualization.

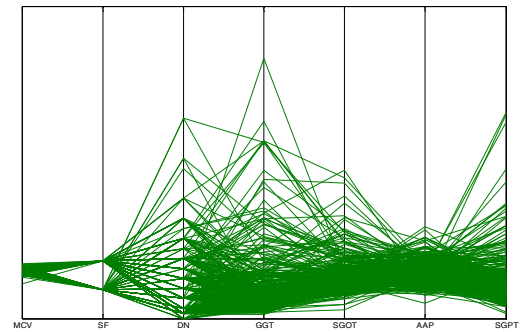


(a) Measurement with NCC

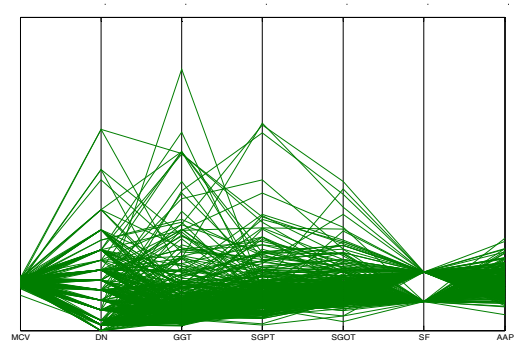


(b) Measurement with PCC.

Figure 1. Axes(dimensions) reordering of Cars dataset in parallel coordinates.



(a) Measurement with NCC.



(b) Measurement with PCC.

Figure 2. Axes reordering visualization of Liver Disorders dataset.

TABLE I. THE COMPARISON OF THE SIMILARITY VALUES USING PCC AND NCC TO CARS DATASET.

PCC / NCC	2	3	4	5	6	7
1	0.7776 / 0.5950	0.7784 / 0.3236	0.8322 / 0.0561	0.4233 / 0.9078	0.5805 / 0.8104	0.5652 / 0.0302
2		0.8429 / 0.5806	0.8975 / 0.5028	0.5046 / 0.8944	0.3456 / 0.0261	0.5689 / 0.6288
3			0.8645 / 0.1313	0.6892 / 0.5223	0.4163 / 0.9544	0.4552 / 0.0104
4				0.4168 / 0.3389	0.3091 / 0.6968	0.5850 / 0.0302
5					0.2903 / 0.9598	0.2127 / 0.0197
6						0.1815 / 0.0117

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