5-2004

Value and Relation Display for Interactive Exploration of High Dimensional Datasets

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Suggested Citation

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Abstract

Traditional multi-dimensional visualization techniques, such as glyphs, parallel coordinates and scatterplot matrices suffer from clutter at the display level and difficult user navigation among dimensions when visualizing high dimensional datasets. In this paper, we propose a new multi-dimensional visualization technique named a Value and Relation (VaR) display, together with a rich set of navigation and selection tools, for interactive exploration of high dimensional datasets. By explicitly conveying the relationships among the dimensions of a high dimensional dataset, the VaR display helps users grasp the associations among dimensions. By using pixel-oriented techniques to present values of the data items in a condensed manner, the VaR display reveals data patterns in the dataset using as little screen space as possible. The navigation and selection tools enable users to interactively reduce clutter, navigate within the dimension space, and examine data value details within context effectively and efficiently. The VaR display scales well to datasets with large numbers of data items by employing sampling and texture mapping. A case study reveals how our proposed approach helps user interactively explore a high dimensional dataset with a large number of data items.

CR Categories: H.5.2 [Information Interfaces and Presentation]: User Interfaces—Graphical user interfaces H.2.8 [Database Management]: Database Applications—Data mining

Keywords: Multi-dimensional visualization, pixel-oriented, multidimensional scaling, high dimensional datasets.

1 Introduction

High dimensional datasets are common in applications such as digital libraries, bioinformatics, simulations, process monitoring, and surveys. Automatic analysis tools are widely used for analyzing high dimensional datasets. For example, automatic dimension reduction approaches, such as Principal Component Analysis (PCA) [9] and Multidimensional Scaling (MDS) [14], are used to project high dimensional datasets into lower dimensional spaces. Subspace clustering algorithms, such as CLIQUE [1], are used to detect data clusters from high dimensional datasets.

However, due to the dimensionality curse [4], i.e., the lack of data separation in a high dimensional space, finding lower dimensional projections, data clusters and other trends from high dimensional datasets is much harder than it is from low dimensional datasets. Thus graphically presenting the high dimensional datasets and then allowing the human to apply his or her perceptual abilities and domain knowledge to make sense of the data is an important approach to both analyzing high dimensional datasets and assessing and understanding the results of automatic analysis tools.

Traditional multi-dimensional visualization techniques, such as glyphs [2], parallel coordinates [8] and scatterplot matrices [5], do not scale well to high dimensional datasets. For example, a dataset containing 200 dimensions will generate star glyphs and parallel coordinates composed of 200 axes and a scatterplot matrix containing 40,000 plots. These large numbers of axes and plots not only clutter the screen but also make it difficult for users to navigate among different dimensions. They make it difficult for users to accomplish exploration tasks such as understanding relationships among dimensions and detecting data clusters and outliers.

In this paper, we propose a new multi-dimensional visualization technique named a Value and Relation (VaR) display. By explicitly conveying the relationships among the dimensions of high dimensional datasets in conjunction with data values, the VaR display greatly helps users grasp the relationships among the dimensions and navigate within the dimension space, as well as detect data clusters and outliers in different subspaces composed of subsets of the dimensions. The VaR display uses pixel-oriented techniques [13] to utilize the screen space efficiently. It also provides a rich set of navigation and selection tools to enable users to reduce clutter and interactively explore high dimensional datasets.

First, by graphically presenting each dimension of a high dimensional dataset as a glyph in a 2D space, the VaR display conveys the relationships among the dimensions through the positions of the glyphs. The positions of the glyphs are generated using Multidimensional Scaling (MDS) [14] according to the pair-wise relationships among the dimensions. MDS is a technique that maps locations in high dimensional space to positions in a low dimensional space. It is widely used in visualization applications to convey relationships among data items within a multi-dimensional dataset. For example, [19] used MDS to map data items in a document dataset to a 2D space and generated a Galaxies display as a spatial representation of relationships within the document collection. The VaR display uses MDS in a different way in that it maps dimensions rather than data items in a dataset to a 2D space according to relationships among the dimensions. In Figure 1a, each dimension of the Sky Server dataset (361 dimensions, 50,000 data items) is mapped to a dot and positioned in the 2D space using MDS. Closely related dimensions have positions adjacent to each other. We call such a display a Galaxies-like display. It reveals the relationships among the dimensions.

Second, besides the relationships among the dimensions, the VaR display conveys values of the data items using pixel-oriented techniques [13]. Pixel-oriented techniques are visualization methods that map values of data items to pixels and arrange pixels to convey relationships. We use pixel-oriented techniques to map values of the data items within a single dimension to pixels and arrange them into a “glyph” (“subwindow”, as termed in other pixel-oriented techniques [10]). For each dimension a glyph can be generated. Then we replace the dots in the Galaxies-like display by their

*This work was supported under NSF grant IIS-0119276.
respective glyphs to produce the VaR display. Figure 1b shows the VaR display of the SkyServer dataset generated by replacing the dots in Figure 1a by glyphs. In such a VaR display, the positions of the glyphs reveal the relationships among the dimensions, while the textures of the glyphs reveal data patterns in the dimensions.

Third, we provide a rich set of navigation and selection tools for the VaR display. Navigation tools help users reduce clutter in the display and interactively explore the dataset. They include interactions such as overlap reduction, zooming and panning, distortion, comparing, and refining. Selection allows human-driven dimension reduction, i.e., users select subsets of dimensions from the VaR display and then a space composed of the selected dimensions can be further explored using the VaR display as well as other multi-dimensional visualization techniques. Automatic and manual selection tools of the VaR display make selection both flexible and easy to use.

The VaR display can be used for the following purposes:

**Visually Exploring High Dimensional Datasets:** The VaR display allows users to interactively explore high dimensional datasets with large numbers of data items. It visually reveals both the data item relationships and dimension relationships within a high dimensional dataset.

**Guiding Automatic Data Analysis:** The VaR display can assist users in (1) assessing and understanding the result of some types of automatic data analysis algorithms and (2) manually tuning the parameters used in those algorithms for better results. For example, by visually presenting the relationships among the dimensions and the values within the dimensions, the VaR display helps users understand the result of an automatic dimension reduction approach. The VaR display also helps users assess the result of an automatic subspace clustering algorithm by visually presenting the clusters.

**Human-Driven Dimension Reduction:** The VaR display allows users to interactively select dimensions of interest and further explore these dimensions using VaR displays as well as other multi-dimensional visualization techniques. For example, a user can select a group of closely related dimensions from the VaR display, project the dataset into the subspace composed of the selected dimensions, and view the projection using parallel coordinates [8].

The remainder of this paper is organized as follows. Section 2 describes how to generate a VaR display and discusses optimization problems in the VaR display generation. Section 3 presents the navigation and selection tools for the VaR display. Section 4 describes the techniques used to scale the VaR display to datasets with large numbers of data items. Section 5 presents a case study of the VaR display. Section 6 reviews related work while Section 7 presents our conclusions and future work.

2 **VaR Display Generation**

The following steps are necessary for generating a VaR display for a high dimensional dataset:

- **Step1:** Build a distance matrix that captures the correlation between each pair of dimensions in the dataset.
- **Step2:** Apply MDS on the distance matrix to get a set of positions in a 2D space, where each position corresponds to a dimension.
- **Step3:** Create a glyph for each dimension: map values of the data items within a single dimension to pixels. Each value is represented by the color of a pixel. Arrange the pixels into a “glyph” that corresponds to the single dimension. Among different glyphs, pixels corresponding to values of the same data items are arranged in the same positions in the glyphs.
- **Step4:** Place the glyphs in their corresponding positions calculated in Step2.

In a VaR display, each glyph represents one dimension of the displayed dataset. The positions of the glyphs reveal the relationships among the dimensions. The colors of pixels within the glyphs reveal data patterns in the dimensions. Thus relationships among dimensions can be examined in detail by comparing the textures of the glyphs.

There are many possible ways to implement the four steps of the VaR display generation. The goal is to find a solution that can provide users with the largest amount of information. The major optimization problems in these steps are how to get a good set of positions for the glyphs and how to arrange the pixels within the glyphs to reveal useful information. These two problems are discussed in the following sections.
2.1 Glyph Position Optimization in VaR Display

To get a good set of glyph positions, we first need to identify the factors that affect the glyph positions. A distance matrix records the correlation between each pair of dimensions in the dataset. There are many different correlation measures [3]. Thus we can get various distance matrices for the same dataset based on the correlation measures chosen. Different distance matrices will lead to different sets of positions generated by MDS. Given that MDS techniques have been widely studied and are mature techniques, we expect that the positions generated by MDS convey the distance matrix with a reasonable quality. Thus the correlation measure is one major factor that affects the positions of glyphs in a VaR display.

Second, one needs to make clear what are good glyph positions. We argue that a good VaR display should have the following properties: it helps users locate similar dimensions, and it helps users identify dissimilar dimensions. According to this argument, the distances between glyphs should be as well distributed as possible in a good VaR display. In other words, the variance, i.e., the average squared deviation from the mean, of the non-diagonal elements in the distance matrix should be as large as possible. Thus the glyph position optimization problem can be expressed as follows: Find a correlation measure so that the variance of all non-diagonal elements of the distance matrix reaches a maximum. We name the variance of the non-diagonal elements the variance criteria of the glyph position optimization problem.

It is impossible to get an optimal solution to this problem since there are infinite possible correlation measures. Thus we use a heuristic approach to calculate a distance matrix based on the fact that in a large-scale dataset, two dimensions might be closely related in part of the data items rather than in all data items. The algorithm for calculating the distance matrix is described as follows:

- **Step1:** Normalize the values within each dimension;
- **Step2:** For each pair of dimensions, build a histogram of the value differences of all data items between the two dimensions. Suppose the number of bins in each histogram is numBins;
- **Step3:** For i = 1 to numBins do:
  - For each pair of dimensions calculate a distance according to its histogram: sort the bins in the histogram according to the number of data items falling into them in a decreasing order. Take the first i bins. The distance is one minus the percentage of data items falling into these i bins.
  - Build a distance matrix Matrix, using the calculated distances. Calculate the variance of its non-diagonal elements Var_i.
- **Step4:** Find the maximum variance Var_j from Var_i (i = 1,...,numBins). Output Matrix_j.

This calculation is based on the assumption that the more data items concentrate in a certain number of bins of a histogram, the closer the two dimensions are. The algorithm loops from 1 to numBins to find the number of bins that generates the maximum variance.

For a large-scale dataset stored in a low-speed memory, computational cost can be ignored with regard to external I/O cost. Thus the time complexity of this algorithm is analyzed as follows: Step1 is a common step needed for most correlation measures and needs two I/Os of the dataset. Step2 requires one I/O of the data set with each data item accessed once to build the histograms. Step2 can be performed in the second I/O of Step1 and thus its cost can be ignored. The dimensionality is usually much smaller than the number of data items in a large-scale dataset. NumBins is usually chosen to be much smaller than the number of data items. Thus the histograms can be stored in a high-speed memory. Thus step3 and Step4 are computations without external I/Os. So the total cost of the algorithm is two I/Os of the dataset.

We have run a series of experiments to compare the variance criteria calculated using the presented algorithm with that calculated using a global Euclidean similarity measure [3]. The experiments were run on 10 real datasets whose dimensionalities range from 4 to 361 and the numbers of data items range from 256 to 95130. The results showed that the variance calculated using the presented algorithm is 45% to 95% larger than that calculated using the global Euclidean similarity measure for the tested dataset in all experiments.

2.2 Pixel Arrangement in Glyphs

Pixel arrangement is an important issue for pixel-oriented techniques [10]. Proposed solutions include spiral arrangement, space-filling curves, and axes techniques among many others [10]. As an
Figure 3: Extent Scaling, Automatic Shifting and Distortion. (a): A VaR display with glyphs seriously overlapped. (b) Overlap is reduced by decreasing the size of the glyphs. (c) Overlap is further reduced by automatic shifting. Notice that several glyphs appear in the center of the display which are previously non-visible in (b) due to overlaps. (d) Some glyphs are enlarged to examine detail within context. The dataset is the Ticdata2000 dataset (86 dimensions, 5,822 data items), which contains information on customers of an insurance company.

initial layout, we used a simple spiral arrangement. Given an order of the data items, the pixels are placed from the center of a square to the outside of the square spirally according to the order.

Initially, we order the data items by their values in one dimension. Such a dimension is called a “base dimension”. Figure 2 shows that selection of the base dimension greatly affects the information conveyed by a VaR display. Patterns existing in dimensions closely related to the base dimension are more explicitly presented than those existing in other dimensions.

In the VaR display, a base dimension is automatically selected when the VaR display is initially presented to the user. The selection criteria is that the base dimension should be a dimension that has the largest number of closely related dimensions so that patterns of the largest number of dimensions is better conveyed in the initial view of a VaR display.

Since “closely related” is a subjective measure, a heuristic approach is used to find the initial base dimension. The base dimension is chosen to be the dimension that has the smallest total distance to all other dimensions in the distance matrix. The user can always select another dimension as the base dimension using the manual pixel reordering tool provided by the VaR display (see Section 3.1).

3 INTERACTIVE TOOLS IN THE VaR DISPLAY

A rich set of navigation and selection tools has been developed for the VaR display. Layer reordering, manual relocation, extent scaling, dynamic masking and automatic shifting help users reduce clutter of the display. Zooming and panning, distortion, comparing, and refining help users learn information about the dataset. While automatic and manual selection tools allow users to perform human-driven dimension reduction by selecting subsets of dimensions for further exploration using the VaR display as well as other multi-dimensional visualization techniques.

3.1 Navigation Tools

Different from all the other pixel-oriented techniques, where each pixel is assigned a unique position on the screen, our VaR display allows overlaps among the glyphs. Overlaps emphasize close relationships among the dimensions because glyphs overlap only if their dimensions are closely related. However, overlaps can prevent a user from seeing details of a glyph overlapped by other glyphs. We provide the following operations to overcome this problem:

Showing Names: By putting the cursor on the VaR display, the dimension names of all glyphs covering the cursor position
are shown in a message bar. Thus a user can be aware of the existence of glyphs hidden by other glyphs.

Layer Reordering: With a mouse click, a user can force a glyph to be displayed in front of the others. In this way he/she can view details of a glyph originally overlapped by other glyphs.

Manual Relocation: By holding the control key, a user can drag and drop a glyph to whatever position he/she likes. In this way a user can separate overlapping glyphs.

Extent Scaling: Extent scaling allows a user to interactively decrease the sizes of all the glyphs proportionally to reduce overlaps, or to increase them to see larger glyphs. Figure 3b gives an example of extent scaling.

Dynamic Masking: Dynamic masking allows users to hide the glyphs of unselected dimensions from the VaR display. In Figure 5, the glyphs of unselected dimensions are hidden using dynamic masking.

Automatic Shifting: This operation automatically reduces the overlaps among the glyphs by slightly shifting the positions of the glyphs. We borrowed a simple distortion algorithm for reducing glyph overlaps from [18] to implement this operation. There are many more advanced overlap reducing algorithms we can use [11, 20]. Figure 3c gives an example of automatic shifting.

Manual Pixel Reordering: As discussed in Section 2.2, we allow users to select a dimension based on which the data items are sorted. Glyphs will have different textures with different base dimensions, thus different patterns of the dataset will be revealed. Figure 2 was generated using manual pixel reordering.

Comparing: It is important to allow a user to compare the values of the data items in one dimension with those in other dimensions so that the relationship between a dimension and other dimensions can be revealed in a more intuitive manner. We allow users to switch to a comparison mode. In comparison mode, except the glyph of the base dimension, the pixels of all other glyphs will be colored according to the differences between the values of the base dimension and their dimensions. Figure 4 shows an example of the comparison operation.

Refining: With a subset of dimensions, refining is an operation that relocates glyphs by MDS using relationships among only the dimensions within the subset while ignoring their relationships to dimensions outside this subset. A display that visualizes glyphs with the relocated positions is called a refined VaR display of this subset of dimensions. A display that visualizes all glyphs of the dataset is called the original VaR display. Refining is different from zooming in that zooming keeps the relative positions of the glyphs in the original VaR display, while refining does not. In the refined VaR display, the positions of the glyphs are decided only by the relationships among the subset of dimensions without being influenced by other dimensions. Thus the glyph positions in the refined VaR display reflect the relationships among the subset of dimensions more accurately than in the original VaR display.

3.2 Selection

Selection tools enable users to select dimensions of interest for further exploration using other multi-dimensional visualization techniques. They can also be used as a filter to reduce the number of glyphs displayed in a VaR display since we allow users to hide glyphs of unselected dimensions using dynamic masking (see Section 3.1). The selection tools we provide to users include an automatic selection tool for closely related dimensions, an automatic selection tool for well separated dimensions, and manual selection.
The automatic selection tool for related dimensions takes a user-assigned dimension and correlation threshold as input. Users can set the assigned dimension by clicking its glyph and set the threshold through a slide bar. The tool automatically selects all dimensions whose correlation measures to the input dimension are smaller than the threshold by traveling through the distance matrix. Using this tool a user is able to select a set of closely related dimensions.

The automatic selection tool for separated dimensions takes a user-assigned dimension and correlation threshold as input and returns a set of typical dimensions that describe the major features of the dataset. The assigned dimension will be included in the returned set of dimensions. Between each pair of dimensions in the result set, the correlation measure is larger than the threshold. For any dimension that is not in the result set, there is at least one dimension in the result set such that the correlation measure between it and the unselected dimension is smaller than the threshold. Using this tool a user is able to select a set of closely related dimensions.

The following algorithm can be used for automatic selection of separated dimensions:

- **Step 1**: Set the assigned dimension as “selected” and all other dimensions as “unselected”.
- **Step 2**: Find all unselected dimensions whose distances to all existing selected dimensions are larger than the threshold. Mark them as “candidate”.
- **Step 3**: If there is no candidate dimension, go to Step 4. Else, set one candidate dimension as “selected” and other candidate dimensions as “unselected”. Go back to Step 2.
- **Step 4**: Return all dimensions marked as “selected”.

Manual selection allows a user to manually select a dimension by clicking its corresponding glyph. The user can unselect a dimension by clicking the glyph again. The combination of manual and automatic selection makes the selection operation both flexible and easy to use.

4 Scaling to Datasets with Large Numbers of Data Items

We have implemented a fully working prototype of the VaR display and its interaction tools in XmdvTool [17], a public-domain visualization system. In order to scale the VaR display to datasets with large numbers of data items, we have integrated sampling and texture mapping techniques into our approach. These techniques allow...
the VaR display to handle datasets with large numbers of data items efficiently.

The prototype stores datasets in an Oracle9i database server and dynamically requests data from the server when needed. When generating a VaR display for a dataset containing a large number of data items, we use a random sampling approach to reduce response time for fetching data items from the server. In particular, users can set a maximum number of data items. When the number of data items contained in a dataset exceeds it, random sampling is performed on the dataset to only fetch the maximum number of data items. Figure 6 shows two VaR displays of a dataset with and without sampling. It can be seen that the corresponding glyphs in the two displays have very similar patterns.

Secondly, in order to reduce the response time of user interactions for large-scale datasets, we store all glyphs as texture objects in OpenGL. Thus unless we need to regenerate the texture of the glyphs, each glyph can be refreshed, repositioned, or resized on the screen by simply redrawing the texture objects, mapping the texture objects to different positions on the screen, or mapping them to areas of different sizes. All these operations can be efficiently performed in hardware.

Both the above two approaches cause information loss in the VaR display. When random sampling is performed, data items not in the sample are not visually presented to the user. When the texture objects are mapped to screen areas that are not exactly their original sizes, magnification or minification happens so that the pixels visualized are only approximations of the original pixels. However, information loss is exchanged for the reduction of clutter in the display and the reduction of response time of user interactions, which are very important for a visual exploration task. Moreover, approximation is usually acceptable in a visualization system. Furthermore, users can always get the information accurately by setting the sampling threshold to a number larger than the number of data items contained in the dataset, and set the size of the glyphs to exactly the size of the texture objects.

5 Case Study

We conducted a case study on the Census-Income-Part dataset, which contains 42 dimensions and 20,000 data items. Its VaR display is shown in Figure 2. We accomplished the following tasks by interactively exploring the dataset through the VaR display:

• We are able to detect groups of closely related dimensions using three methods: (1) looking for glyphs clustered together in the VaR display; (2) looking for glyphs with similar patterns; (3) selecting dimensions closely related to a dimension of interest using the automatic selection tool for related dimensions. Using these three methods together helps us get results quickly and intuitively. Figure 2b shows a group of closed related dimensions in the bottom left of the display. By checking the dimension names we found that these are all dimensions recording people’s migration and moving status in the last year.

• We are able to find data clusters in a subset of the dimensions from similar patterns of the graphs. For example, in Figure 2b, within each glyph in the bottom left of the display, pixels in the center area have different color from that in the outer area. Then we determine that data is divided into two clusters in those dimensions, which are the people who did not move in the last year and people who moved in the last year.

• We are able to find well separated dimensions of the dataset using three methods: (1) looking for glyphs well distributed in the display; (2) looking for glyphs with significantly different patterns; (3) selecting well separated dimensions using the automatic selection tool for separated dimensions. Using these three methods together helps us get results quickly and intuitively.

• We are able to find dimensions with special patterns. For example, there were several dimensions with lots of values mapped to red in the VaR display. According to the color code we found that those dimensions contain a high rate of missing values. We then can remove them from the display.

Through the case study we found that the VaR display and its navigation and selection tools could help users discover interesting patterns in a high dimensional dataset with a large number of data items effectively and efficiently.

6 Related Work

Multidimensional Scaling (MDS) [14] is an iterative non-linear optimization algorithm for projecting multi-dimensional data down to a reduced number of dimensions. It is often used to convey relationships among data items of a multi-dimensional dataset. In our
approach, MDS is used in a different way in that it is used to convey relationships among dimensions rather than data items.

Pixel-oriented visualization techniques [13, 10] are a family of multi-dimensional display techniques that map each data value to a pixel on the screen and arrange the pixels in such a way as to convey relationships. They generate condensed displays and may reveal clusters, trends, and anomalies visibly. The VaR display is different from existing pixel-oriented visualization techniques because it uses positions of the subwindows (glyphs in the VaR display) to accurately convey the relationships among the dimensions. In addition, many interactions of the VaR display, such as extent scaling and comparing, have not previously been applied to pixel-oriented techniques.

The VHDR [22] and DOSFA approaches [21] explicitly convey the relationships among the dimensions of a high dimensional dataset using a dimension hierarchy. They allow users to interactively navigate and select dimensions from it. The VaR display is different from them in that it uses MDS to convey the relationships among the dimensions in a richer, more accurate fashion. In addition, the VaR display conveys values of data items, while VHDR and DOSFA do not.

Sampling has been used in pixel-oriented techniques. VisDB [12] allows users to interactively change the number of data items displayed on the screen using sampling. The VaR display uses sampling in particular to limit the number of data items fetched when generating the glyphs in order to reduce I/O cost.

7 CONCLUSION

The major contributions of this paper are:

- A new method for the display of high dimensional datasets, the VaR display, has been proposed and developed. The VaR display not only conveys values of the data items to the users, but also explicitly conveys relationships among the dimensions of a high dimensional dataset.
- A rich set of navigation tools for the VaR display has been implemented to allow users to interactively explore the dataset displayed. These interaction tools help users identify patterns hidden in a high dimensional dataset effectively and efficiently.
- Selection tools for the VaR display have been developed to enable users to interactively select dimensions of interest from the VaR display for further exploration.
- Criteria and algorithms for the distance matrix generation and the base dimension selection have been created for generating a relatively informative VaR display among many possible ones.
- Sampling methods and texture mapping have been used to enable the VaR display to efficiently scale to datasets with large numbers of data items.

In the future, we plan to explore different pixel arrangement approaches for constructing the glyphs of the VaR display, develop techniques to allow users to compare data between values of a group of dimensions with other dimensions rather than a single dimension, and evaluate the effectiveness and efficiency of the proposed approach using more formal experiments and user studies.

8 ACKNOWLEDGMENTS

We gratefully thank Dr. Daniel A. Keim, who gave many valuable suggestions for this work.

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