Evaluating Reordering Strategies for Cluster Identification in Parallel Coordinates

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Abstract

The ability to perceive patterns in parallel coordinates plots (PCPs) is heavily influenced by the ordering of the dimensions. While the community has proposed over 30 automatic ordering strategies, we still lack empirical guidance for choosing an appropriate strategy for a given task. In this paper, we first propose a classification of tasks and patterns and analyze which PCP reordering strategies help in detecting them. Based on our classification, we then conduct an empirical user study with 31 participants to evaluate reordering strategies for cluster identification tasks. We particularly measure time, identification quality, and the users’ confidence for two different strategies using both synthetic and real-world datasets. Our results show that, somewhat unexpectedly, participants tend to focus on dissimilar rather than similar dimension pairs when detecting clusters, and are more confident in their answers. This is especially true when increasing the amount of clutter in the data. As a result of these findings, we propose a new reordering strategy based on the dissimilarity of neighboring dimension pairs.

CCS Concepts

- Human-centered computing → Empirical studies in visualization;

1. Introduction

Parallel coordinates plots (PCPs) [Ins85, Ins09b] are a popular and well-researched technique to visualize multi-dimensional data. Dimensions are represented by vertical, equally spaced axes. Data records are encoded by polylines, connecting the respective values on each axis. PCPs have been applied to practical applications of various domains [JF16], such as finance [AZZ10], traffic safety [FWR99], and network analysis [SC\(^\ast\)05]. As discussed by Andrienko and Andrienko [AA01], PCPs are suited for a multitude of analysis tasks, such as cluster, correlation, and outlier analysis.

Compared to other visualizations for multi-dimensional data (e.g., RadVis [HGM\(^\ast\)97], MDS and PCA projections, scatter plots, and scatter plot matrices), PCPs have the advantage to trace data records and patterns across a large set of dimensions. Empirical studies have shown that PCPs outperform scatter plots in clustering tasks, outlier, and change detection [KAC15], but are less suited for correlation analysis [LMW10, HYFC14] and value retrieval [KZZM12].

A major challenge of visualizations is visual clutter, which influences the perception of visible patterns [SKKAJ15]. This problem is particularly given in PCPs, as line crossing and overplotting distort salient structures. Therefore, the community has proposed a multitude of enhancements, such as sampling [ED06], edge bundling [MM08], interactive highlighting [MW95], and the usage of transparency [JLJC05] to reduce the impact of visual clutter.

The ordering of axes plays a fundamental role in the design of a PCP and has a strong effect on the overall pattern structure [JJ09]. In contrast to data preprocessing, sampling, dimension filtering, and other enhancements, reordering does not remove data from the PCP [PWR04, PL17], but changes the visual structure among neighboring axes. Depending on the user’s analysis goal, some patterns are more interesting than others [DK10]. As a result, more than 30 different ordering strategies have been developed by the community to support a multitude of tasks. Some of these strategies group similar dimension pairs [ABK98], try to avoid line crossings [DK10], or put the most important dimensions first [YPWR03]. However, our community lacks empirical guidance and recommendations for
choosing an appropriate strategy for a given task [BBK*18]. In this paper, we address this limitation by summarizing the state-of-the-art in axes reordering strategies, as well as presenting a first empirical user study that measures the performance of two ordering methods for cluster identification in PCPs. Our study focuses on cluster analysis as the majority of ordering strategies are designed for this task.

We claim two main contributions. First, we provide guidance in selecting reordering strategies based on their intended patterns. Many existing algorithms follow similar concepts but differ in their implementation. To support users, we introduce a classification of the existing layout algorithms, group them according to their inner workings, and summarize their intended patterns and meta-characteristics. For more practical support, we implemented a set of 14 strategies in JavaScript and made them along with the source code available on our website for testing: http://subspace.dbvis.de/pcp.

Second, we measure the performance of two reordering strategies for cluster identification tasks by an empirical user study with 31 participants. We realized that the often proposed similarity-based axes arrangement (e.g., [ABK98, YPWr03, AdO06]) is not always the most effective solution to identify clusters. As shown in Figure 1, arranging axes with a high dissimilarity next to each other produces more salient clusters, in particular in cluttered and noisy datasets. A reason for this effect is that lines with strong slopes are moving closer together, making clusters visually more prominent [PDK*19]. To find out whether this arrangement is more useful than a similarity-based layout, we conducted a user study and measured performance with respect to cluster quality, completion time, and users’ confidence using synthetic and real-world datasets. Our results show that participants tend to focus on dissimilar axes pairs when selecting clusters and are more accurate and confident when doing so.

As a secondary contribution, we provide a benchmark dataset with 82 synthetic and real-world datasets for clustering analysis. For reproducibility, we make all our material and results, statistical analysis, and source code publicly available at https://osf.io/zwm69.

The remainder of this paper is structured as follows: In the next section, we summarize important related work. Then, in Section 3, we survey existing reordering strategies for PCPs and classify them based on their intended patterns and inner workings (first contribution). Afterwards, in Section 4, we describe our user study design and report the statistical analysis results in Section 5 (second contribution). Finally, we discuss our findings and derive design considerations for axes orderings in cluster identification tasks.

2. Background and Related Work

In the following, we summarize the challenges of axes reordering, the results of existing user studies, and the relation of automatic ordering to interactive and semi-automatic analysis support.

2.1. Challenges of Axes Reordering of Parallel Coordinates

Linear ordering of an n-dimensional dataset in PCPs faces two main challenges. First, computing and evaluating all dimension permutations is computationally expensive. Ankerst et al. [ABK98] show that the ordering of axes according to some useful objective function is NP-complete. Therefore, the exhaustive search for a useful ordering is tedious, even for a modest number of dimensions [PWR04]. Second, the usefulness of a particular ordering highly depends on the analysis task of the user [DK10, PL17], and is influenced by the complexity of the data [TAE*11]. More importantly, optimizing the axes ordering to highlight a particular pattern may even obstruct other patterns [JFJ09], which are of relevance in a different scenario. Therefore, it is vital to carefully choose an appropriate strategy to arrange the axes in parallel coordinates.

More than 30 reordering strategies have been developed (see Section 3), many of which follow similar concepts but differ in their implementation affecting, for example, the runtime and quality of the results. Quality metrics and layout algorithms for PCPs have been summarized before: Heinrich and Weiskopf [HW13] give a comprehensive overview of the state-of-the-art for PCP research, including manual and automatic reordering approaches. Bertini et al. [BTK11] and Behrisch et al. [BBK*18] summarize quality metrics to optimize the visual representation. Ellis and Dix [ED07] discuss reordering from a clutter perspective. While Behrisch et al. [BBK*18] group the quality metrics by their analysis task, the literature still misses a summary of the different PCP patterns and a discussion on which reordering algorithms favor or avoid particular patterns [TAE*11]. In our paper, we close this gap by introducing a classification along with a characterization of the reordering algorithms.

2.2. Evaluation of Axes Reorderings and Empirical Studies

There is a lack of empirical studies to measure the performance of specific axes orderings for different analysis tasks [JFJ16]. Most strategies are “evaluated” using examples of synthetic or real-world data (see Table 1) instead of comparing it to previous approaches. Exceptions are the works by Ferdosi & Roerdink [FR11] and Tatu et al. [TAE*11], which compare the resulting orders with competing approaches. However, no feedback from real users is provided.

Many reorderings claim to be useful for cluster analysis, but we do not know yet which patterns are most effective in identifying clusters. There is no user study that compares different reorderings for cluster identification in particular or different analysis tasks in general. Therefore, we want to push PCP reordering towards an empirically-driven research field by evaluating two axes reordering techniques for cluster identification. The works most closely related to ours are the empirical studies by Holten & van Wijk [HV-W10] (measuring response time and cluster identification correctness for nine PCP variations), Kanjaniabose et al. [KAC15] (measuring response time and clustering accuracy in PCP, scatter plots, and classical tables), and the study by Johansson et al. [JFC08] evaluating clutter threshold for the identification of patterns. However, none of these studies consider different axes orderings as an independent variable.

2.3. Relation to Interactive and Semi-Automatic Analysis

Besides axes reordering, countless enhancements have been developed to support the understanding of patterns in parallel coordinates. A comprehensive overview is out of the scope of this paper but can be found in the surveys by Ellis & Dix [ED07], Bertini et al. [BTK11], Heinrich & Weiskopf [HW13], and Behrisch et al. [BBK*18]. Many techniques involve users within an interactive exploration workflow or combine the representation with automatic algorithms for pattern detection. Examples are the usage of clustering algorithms [FWR99, JLIC05, Mou11], automatic sampling techniques [ED06], and interactive highlighting [MW95]. Inselberg [Ins09a], and Hurley & Oldford [HO10] propose to clone
and arrange dimensions such that all pairwise permutations are visible, similar to a scatter plot matrix. Based on this initial view, the user can then start the exploration.

While the usefulness of such interactive and visual analytics approaches have been shown in many user studies, they are facing two challenges: First, most algorithms rely on sensitive parameters which influence the quality of the result. For example, k-means clustering [HKP11] requires the number of clusters as user input, which is typically unknown for a new dataset. Second, interactive exploration and highlighting are difficult if users do not know what they are searching for, and the initial configuration of a PCP does not show (parts of) interesting patterns. Often, this results in trial-and-error interactions, in which patterns are only detected ‘by accident’. This is particularly true if the dataset contains a large number of dimensions, and relevant patterns only exist in smaller subspaces.

Therefore, we need methods to give analysts good starting conditions for their (interactive) analysis. Hereby, an important aspect is the arrangement of axes, as it significantly changes the visual patterns among neighboring axes [JJ09]. In our paper, we provide a categorization of reordering algorithms and their intended patterns, which helps analysts to make an educated selection.

3. Classification of Reordering Strategies
This section addresses two questions: Which patterns are emphasized by which reordering strategy? And which algorithms have been implemented to solve the reordering problem? Before answering these questions, we provide an overview of important patterns.

3.1. Visual Patterns
Figure 2 shows five groups of the most common patterns in parallel coordinates and their representation in scatter plots:

Clusters & Neighbors A – E. Typical cluster structures show one or more groups of dense lines in a similar direction. While A & B seem similar in scatter plots, the visible structure in PCP differs significantly. C shows clusters that change their density (cluster compactness) and D, a cluster that splits up into sub-clusters.

Structures, preserving neighborhood information, are a special case of clusters. A (small) set of data records similar (close) to each other in one dimension are also similar in the neighboring dimension, which results in groups of parallel lines E.

Correlations F – H. Positive and negative correlations look similar in a scatter plot. However, the PCP patterns differ: lines are parallel for positive F, and in a star-like pattern for negative correlations H. Variations of non-linear correlations may look different in both scatter plots and PCPs. H shows only an example as the pattern depends on the type and degree of change in both dimensions.

Outliers I. Outliers squeeze the majority of PCP lines together, resulting in a cluster-like pattern, hiding the underlying structure.

Dimension Properties J – K. show patterns of dimensions, ordered by variance and skewness. The lines’ slope indicates whether patterns stay consistent (parallel) or change across axes.

Clutter & Noise. Randomly distributed data without a clear pattern is considered noise or clutter in the data. The lines in the PCP cross without any particular structure M. The fan pattern L describes a cluster transitioning into clutter, a special case of density change C.

Our selection of patterns is based on the work by Dasgupta & Kosara [DK10], Wegman [Weg90], Heinrich & Weiskopf [HW13, HW15], and Zhou et al. [ZYQ’08]. The cluster variations (i.e., patterns A – D) are inspired by Pattern Trails [JHB’17], which introduces a taxonomy of pattern transitions between multi-dimensional subspaces. These patterns can be adapted to PCP, as two neighboring axes show a transition between one-dimensional subspaces. Finally, we add variance J and skewness K, which is produced by the algorithms described in [LHZ16, SCC’18, YPWR03]. We limit our patterns to 2D PCPs and ignore patterns in 3D PCPs (e.g., discussed in [PL17, AKSZ13]). We also consider only patterns among the two axes. Multi-dimensional patterns can be achieved by concatenating multiple two-dimensional patterns.

3.2. Ordering Strategies
To find ordering strategies, we took the 502 references of recent state-of-the-art reports [HW13, JF16, BBK’18] and combined it with 497 papers resulting from a search on the ACM, IEEE Xplore, EG, and DBLP digital library (see keywords and details in the supplementary material). We recursively scanned references and excluded papers that (1) did not propose an automatic axes ordering strategy (e.g., purely interactive approaches), (2) “just” apply a reordering method which has been proposed before, or (3) approaches which do not focus on “standard” parallel coordinates (e.g., 3D PCPs). Using this approach, we collected 18 papers with 32 different strategies.

Table 1 summarizes all reordering strategies, grouped by their ordering concept: strategies transforming the reordering into an optimization problem (Section 3.3), implementing efficient or sophisticated algorithms (Section 3.4), and approaches focusing on properties of single dimensions (Section 3.5). For each approach, we indicate the favored patterns, the involved axes, and the performed evaluation to show the usefulness (see caption of Table 1 for details).

3.3. Optimization Problem and Objective Functions
The largest group of reordering strategies transforms the axes arrangement into an optimization problem. These approaches measure the quality of a particular ordering by an objective function, which is then either minimized or maximized by an optimization algorithm.
Table 1: Reordering Classification summarizing the inner workings of reordering strategies for parallel coordinates. For each technique, we mark if it favors or avoids a particular pattern, if present in the data. Empty cells mean that the technique is not designed for this pattern and produces/avoids it primarily by change. Approaches are grouped by their concept and sorted according to the similarity of patterns that they favor and avoid. Additionally, we indicate the number of dimensions that are taken into account for the reordering and mark techniques which can be combined with dimension filters and subspace analysis. Finally, we mark the evaluation type used in the paper. Due to space limitations, we only show the name of the first author.

Patterns: algorithm favors ⬤ or avoids ⬤ pattern, or it depends on data properties and algorithm parameters ⬤.
Axes considered for ordering: each dimension separately ( ), two neighboring dimensions ( ), or the majority of dimensions ( ).
The technique can be combined with: dimension filters (DR) and subspace analysis (G).
Evaluation: case study or example ( ), comparison with other techniques ( ), and empirical study ( ).

| Reordering Technique | A | B | C | D | E | F | G | H | I | J | K | L | M | Axes | Dim. | Eval. |
|----------------------|---|---|---|---|---|---|---|---|---|---|---|---|---|------|------|-------|
| Tatu (no label) [TAE+11] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Tatu (given label) [TAE+11] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Long (class consist.) [Van15] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Zhou (cluster trace) [ZYCY18] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Peltonen (neighbor) [PL17] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Dasgupta (overpl.) [DK10] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Dasgupta (parall.) [DK10] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Ankerst (similar) [ABK98] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Yang (similarity) [YPWR03] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Xiang (clus. interac.) [XFJ12] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Artero (clutter) [AdOL06] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| ★ Blumenschein (dissimil.) | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Dasgupta (cross.) [DK10] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Dasgupta (angle) [DK10] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Dasgupta (mut. i.) [DK10] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Makwana (struc.) [MTJ12] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Peng (outlier) [PWR04] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Dasgupta (entropy) [DK10] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
| Dasgupta (diverg.) [DK10] | ⬤ | ⬤ | ⬤ | | | | | | | | | | | | | |
3.3.1. Objective Functions Measuring Cluster Structures

Tatu et al. [TAE∗09, TAE∗11] argue that clusters consist of lines with a similar position and direction (patterns A, B, and D). The authors take a rendered image of a PCP and apply a Hough space transformation [Hou62]. Each PCP line segment is mapped into one point within the Hough space. The point’s location represents the position and slope of the line segment. The objective function measures dense areas (clusters) of points in the Hough space. Long [Van15] first computes a centroid for all given clusters. Then for each data record, the nearest centroid is identified (using the area between the lines as similarity function), and the objective function measures the ratio of correctly classified records. Cluster patterns A and B are highlighted, while a cluster split D is avoided. Zhou et al. [ZYYC18] aim at clusters that can be followed across neighboring axes (A and B). They compute a hierarchical clustering on every dimension and use the cluster similarity as quality. Dasgupta & Kosara [DK10] introduce seven different metrics, known as pargnostics. A metric aiming for clusters like A and B is overplotting. It measures the number of pixels that are not visible due to overlapping lines. When maximizing this measure, there is a high information loss, but a high-density of lines, i.e., clusters. Finally, Xiang et al. [XFJ12] try to avoid intersecting clusters B by measuring the crossing of clusters among axes. This results in horizontal cluster structures A.

Peltonen & Lin [PL17] aim to preserve the neighborhood distribution of records (pattern B). The objective function measures the similarity of nearest neighbors for all data records across two dimensions. Clusters like A and B are a special case of neighborhood relationships and are therefore considered as well.

3.3.2. Similarity-based Metrics for Clusters and Correlation

The main idea of the following approaches is to arrange similar dimensions next to each other. This results in cluster- and correlation patterns. The definition of similarity differs across the techniques. Ankerst et al. [ABK98] use a Euclidean distance and Pearson correlation for the similarity computation. The approach by Yang et al. [YPWR03] follows the same idea. However, they structure the dimensions into a hierarchy using a hierarchical clustering algorithm to highlight also clusters in subspaces of the dataset. The hierarchical structure also helps to speed up the computation time, as each subtree can be sorted independently. Depending on the similarity function, and whether the objective function is minimized or maximized, these approaches aim for the patterns A, B, F, G, and H.

Other metrics try to order axes such that lines are most parallel or diverging a lot. These patterns can help to identify correlations, but may also favor clusters to some extent. Artero et al. [AdOL06] propose the total length of poly-lines as metric for pattern F. Similarly, there are four pargnostic [DK10] measures: (1) Maximizing the number of line crossings to identify inverse relationships G in the data. (2) Maximizing the angle of crossings. (3) Maximizing parallelism, resulting in less cluttered PCPs, which highlight positive correlations F. (4) Maximizing the mutual information, which measures the dependency between variables, i.e., optimizing for positive F, negative G, and non-linear correlations H.

3.3.3. Objective Functions for Clutter and Outliers

The pargnostic metric maximizing divergence results in fan pattern L, which helps to identify cluster-to-noise relationships. Maximizing the entropy of neighboring axes corresponds to a high information density, highlighting many line crossings and inverse relationships. The metric does not favor specific patterns, but results in busy, but very readable charts, according to the authors [DK10]. The metric by Makwana et al. [MTJ12] differs from previous metrics. The authors propose to order dimensions such that neighboring axes contain lines with different slopes, resulting in cluttered M PCPs.

Peng et al. [PWR04] interpret outliers as data points that do not belong to a cluster. They measure the ratio of outliers against the number of data points. When maximized, outliers are highlighted (pattern I), when minimized, outliers will not be highlighted.

3.3.4. Optimization Algorithms for Objective Functions

Except for [AdOL06], all approaches measure the quality between neighboring axes || and use the average as the objective function. To minimize or maximize this function, various heuristics are applied: Random swapping (particularly useful for very large datasets) [YPWR03, PWR04], Ant-optimization [ABK98], A∗Search [TAE∗09, TAE∗11], Nearest-neighbor-based [PWR04], Branch and bound optimization [DK10, MTJ12], Non-linear optimization algorithm [PL17], and Backtracking [ZYYC18].

3.4. Reordering by Algorithms

The second class of strategies arranges dimensions based on layout algorithms. Compared to optimization procedures, this has two advantages: (1) Algorithms which approximate the understanding of an objective function, lead to more efficient but potentially less accurate results (e.g., [LHH12, AdOL06, JJ09]). (2) Objective functions are typically defined only between neighboring axes. Using more advanced algorithms (e.g., based on subspace clustering) lead to PCP, which aims for higher-dimensional patterns [FR11].

3.4.1. Algorithms for Efficient Reordering

Artero et al. [AdOL06] and Johansson & Johansson [JJ09] speed up the similarity and correlation-based axes arrangement, originally presented by Ankerst et al. [ABK98]. Both algorithms are identical, except for the similarity function. Artero et al. use a Euclidean distance, Johansson & Johansson, a Pearson correlation coefficient. The algorithm starts with the most similar dimension pair in the center of the PCP. Iteratively, the next most similar dimension is appended to the left or right side. While this approach is efficient, it also has the advantage that the most salient structure (the most similar dimensions) typically ends up close to the center of the PCP, which users are most attracted to [NVE∗17]. Lu et al.’s approach [LHH12] orders dimensions based on correlation. They use the nonlinear correlation coefficient (NCC), which is sensitive to any relationship F–H (not only linear ones) and can be used for partial similarity matching as well [ABK98]. The proposed algorithm combines the ordering by (non-linear) correlations together with an importance driven arrangement. The first (left) axis in the PCP is chosen based on the highest singular value after a singular value decomposition (SVD, highest contribution of the dataset). Afterwards, all dimensions are arranged from left to right according to their similarity of the NCC. The approach by Huang et al. [HHJ11] maximizes the uniform line crossings of clusters. Their approach is based on Rough Set Theory [Paw12], and the algorithm sorts the dimensions based on alternating sizes of high and low cardinality of the equivalence classes, leading to cluster patterns A–C.

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3.4.2. Subspace Algorithms for Higher-dimensional Structures
Ferdosi & Roerdink [FR11] use a subspace search algorithm [FBT+10] to identify higher-dimensional clusters with patterns \(\mathcal{A} - \mathcal{D}\). The quality of one subspace is based on a density distribution. Subspaces containing multiple clusters that are clearly separated are considered of high quality. First, the algorithm computes all one-dimensional subspaces and arranges the one with the highest quality on the very left of the PCP. Afterwards, all two-dimensional subspaces, which contain the first subspace, are computed, and the highest rank is attached as the second axis. The algorithm continues until all dimensions are part of the PCP, or no more subspace can be computed. Johansson & Johansson [JJ09] apply the MAFIA algorithm [NGCO1], resulting in a set of subspaces, along with cluster structures and quality measures. The ordering algorithm then finds the longest sequence of connected variables shared by all detected subspace clusters. It starts with all dimensions of the first subspace (no specific ordering). Further subspaces are iteratively added based on their quality, but only if they share a substantial set of dimensions with the current PCP. The authors use the same algorithm to identify patterns with (multi-dimensional) outliers (pattern \(\mathcal{D}\)).

3.5. Reordering by Dimension-wise Quality Metrics
The third group of reordering techniques computes a quality for each dimension separately (\(1\)) and sort the axes accordingly. Assuming the quality can be computed efficiently, reordering can be done in linear time. The techniques can also be extended by dimension filtering (e.g., considering only dimensions with a quality above a threshold). Relations between dimensions are not considered. Therefore, patterns may be scattered in different parts of the PCP [PL17].

Lu et al. [LHZ16] sort the axes based on each of their contributions to the dataset. They compute an SVD and sort the dimensions according to their singular values. Yang et al. [YPWR03] propose a similar approach but sort the dimensions by variance. Both reorderings result in similar patterns (\(\mathcal{D} - \mathcal{D}\)). However, Lu et al.’s approach takes the distribution of the entire dataset into account.

Schloerke et al. [SCC18] propose three different dimension metrics: (1) They use skewness for reordering, resulting in a \(\mathcal{D}\) pattern. (2) The dimensions are sorted by one of the Scagnostics [WAGO5] measures. In particular, the Outlying measure is useful to highlight outliers in the data (pattern \(\mathcal{D}\)). (3) Finally, the authors order the dimensions such that existing clusters or classes are separated as well as possible. They compute an ANOVA on every dimension based on a given set of class labels and order the dimensions based on the F-statistic. Intuitively, the dimensions are ordered according to how well the given clusters are separated (patterns \(\mathcal{A} - \mathcal{C}\)).

3.6. Summary
In Table 1, we provide an overview of 32 different reordering approaches to arrange the axes of parallel coordinates. During our analysis, we made a few observations: (1) Many reordering algorithms follow similar concepts, but differ in their implementation and the applied metric. The main reason for this is that axes reordering is computationally complex, and more efficient approaches are necessary for interactive applications. (2) There seems to be a different understanding of the most important area in a PCP. While some reordering approaches try to put the most important dimensions upfront, others try to arrange them in the center. This is in line with the study by Netzel et al. [NVE+17], who found out that people pay the most attention to the center part of a PCP. (3) The evaluation of novel reordering algorithms is primarily achieved by use cases and example applications. We are not aware of empirical user studies that compare different orderings for a particular analysis task. With our paper, we want to close this gap and provide the first empirical study to evaluate ordering approaches for a particular analysis task.

4. User Study Design: Reordering for Cluster Identification
Our reordering classification in Table 1 reveals that the majority of strategies are designed to support cluster analysis. Therefore, we select this task as the focus of our user study. In particular, we want to assess the performance of cluster identification, as this is the foundation for more sophisticated clustering analyses.

For cluster analysis, similarity-based layouts are proposed most often. Clusters, if present, can be followed across many axes, as algorithms try to minimize their variance. However, this strategy does not necessarily highlight clusters. This is especially true if the dataset contains noise or clutter, as shown in Figure 1a. While we can identify the clusters, they are visually less salient. In this paper, we define the term clutter as data records that do not contribute to a particular pattern (e.g., randomly distributed), often also called noise. Cluttered datasets often end up in visual cluttered PCP due to many line crossings and overplotting.

Due to experiments with our implemented reordering algorithms, we realized that polylines and clusters with strong slopes are visually more prominent than horizontal ones. There are two reasons, as discussed by Pomerence et al. [PDK+19]: (1) With an increasing slope, the distance between polylines decreases, and less whitespace (background) is visible. Hence, neighboring lines have higher contrast. (2) Compared to horizontal lines, diagonal lines need more pixels to encode a single data point, resulting in a low data-to-ink ratio [Tuf01]. Both geometric effects make sure that neighboring lines are more easily perceived as a group or cluster. Interestingly, strong slopes are produced when dimensions are ordered by dissimilarity. An example can be found in Figure 1c. It shows the same data as in 1a, but with strong slopes due to reordering. Often this results in a zig-zag-like pattern, which makes the visual representation more complex but also ends up in more salient cluster structures.

4.1. Hypotheses
We address the question, ‘whether there is a difference between a similarity-based (\(\mathcal{S}\)) and dissimilarity-based (\(\mathcal{D}\)) axes ordering for a cluster identification task’. If yes, ‘which ordering should be used, and why?’ As the majority of real-world datasets contain noise and clutter, we also want to investigate its influence generally, and in combination with the axes ordering. Hence, we analyze two independent variables: ordering method and clutter level.

To measure the performance, we use three dependent variables: (i) time to identify clusters, (ii) quality of manually selected clusters based on similarity to ground truth clusters, and (iii) the confidence of the users after the cluster identification. Additionally, we analyze axes-pairs which help to identify the clusters. In particular, we investigate whether users select clusters in similar or dissimilar axes pairs. For our study, we formulate the following three hypotheses:

H1: With an increasing amount of clutter, the cluster identification performance drops (independent of the ordering) as cluster structures
are less salient in the PCP plot. Therefore, we expect users to be (a) slower, (b) less accurate, and (c) less confident.

H2. Without clutter, users perform better in a cluster identification task when the axes are ordered by SIM instead of DIS as clusters can be followed more easily. In particular, we expect users to be (a) faster, (b) more accurate, and (c) more confident with SIM.

H3. With clutter, users perform better in a cluster identification task when the axes are ordered by DIS instead of SIM as clusters are visually more prominent. In particular, we expect users to be (a) faster, (b) more accurate, and (c) more confident with DIS.

4.2. Benchmark Dataset and Ground Truth

To evaluate our hypotheses, benchmark datasets with ground truth information and increasing clutter levels are needed. We are not aware of such datasets for a cluster identification task. Therefore, we developed our own benchmark, consisting of ten popular real-world, and 22 synthetically created datasets along with the ground truth information. We make our dataset available in order to overcome the limitation of publicly available benchmark datasets [SNE*16] and to support the evaluation of PCP enhancements and reordering techniques in the future. For comparison, we also present a PCP with each dataset and reordering strategy in the supplementary material.

Synthetic datasets. We limit the dimensionality of all synthetic datasets to eight. This allows us to create complex cluster structures while keeping the expected time for the study in a reasonable time frame. We alternated the number of clusters between one and four and varied the structures of the clusters – ranging from linear clusters towards a high variance on all scales of the different axes.

Using the PCDC tool [BHvL12], we manually created 24 base datasets (1,2,3,4 clusters × 6 variations) which fulfill the following properties: (i) clusters are clearly visible and separated from each other, (ii) there is only one clustering result per dataset, (iii) each cluster is present in all eight dimensions, and (iv) no outliers are added as they would distort the existing patterns [AA01]. In up to two dimensions, we merged two or more clusters such that participants need to investigate all dimensions to identify a cluster. To make the clusters comparable across datasets, we kept the cluster size constant with small randomization in the range of 45–50 data points and vary the diameter of every cluster in each dimension randomly in the range 0.15–0.30. All dimensions are normalized in 0.0–1.0.

Next, we designed different clutter levels. Pomerenke et al. [PDK*19] show that random clutter (randomly and equally distributed records in all axes) produces visible patterns in PCPs which look similar to clusters (Ghost clusters). In order to not accidentally include ‘fake patterns’ in our dataset, but also be fair w.r.t. random clutter, we use a mixture of 30% random and 70% linear clutter (for every record: uniform and random distribution in one dimension 0–0.15 in all other dimensions). Using several pilot experiments, this setting seemed to be complex enough, but also without any undesired patterns. For each base dataset, we created two copies with different clutter levels, one with 150 (150N), one with 300 data points (300N). We used the same clutter datasets for all base datasets to make them comparable and ensure we do not encode additional patterns in some of the datasets. After finalizing all 72 datasets (24 base datasets ×{ON,150N,300N}), we randomized the order of the records to remove potential effects in the drawing process.

Real-world datasets. We added ten frequently used datasets to see the performance in real settings. We selected the datasets based on common usage in PCP reordering (i.e., by choosing datasets used in the techniques described in Table 1). Hence, the number of dimensions and records differ compared to synthetic datasets. Dimensions range between 4–13, and the number of records between 32–515. Examples are the wine, mt-cars, and ecoli dataset. If present, we removed categorical dimensions and outliers. We used Ward’s method [W63] to retrieve a hierarchical clustering and a visual inspection to determine the clusters in the data.

4.3. Implementation

To compare the ‘optimal’ SIM and DIS layout, we used Ankerst et al.’s reordering algorithm [ABK98] with an exhaustive search to find the axes ordering. For the SIM layout, we used the Euclidean distance and minimized the sum of distances. For DIS, we used the same algorithm but maximized the distances. We pre-computed the orderings for all datasets in advance. To run the study, we developed a web application that is available at http://subspace.dbvis.de/pep-study. The parallel coordinates plots have a size of 960 × 500 pixels and use color for the polylines to separate them from the axes which are colored in black. We did not add any design variations to the chart (i.e., transparency, or edge bundling) to avoid confounding factors.

4.4. Tasks and Data Randomization

Our study consisted of 21 trials per participant, which are grouped into three tasks that build on top of each other. The tasks were executed in increasing difficulty: Tasks 1, 2, and 3. Between two trials of a task, we showed a white screen with the term ‘break time’, and participants had to click a button to continue with the next trial.

4.4.1. Task 1 (Similarity of Axes-Pairs)

We wanted to find out which visual structures support users in a cluster identification task. In particular, we were interested whether users find neighboring axes with a high similarity or dissimilarity more useful. In each trial, we showed the participants a PCP in which the number of clusters had to be counted. Users selected the number which they identified using four radio buttons (i.e., 1, 2, 3, 4) and a ‘can’t tell’ option. After the selection was confirmed, we showed a single radio button between each neighboring axes (see Figure 3 left) and asked the participants to select the pair which supported them best. Only one pair could be selected.

Randomization. We randomly picked three synthetic datasets with a different number of clusters. In the first trial, we showed ON clutter, in the second 150N, and finally 300N (increasing difficulty). As we are interested in whether participants prefer (dis-)similar neighboring axes, we arranged dimensions such that the PCP contains both similar and dissimilar axes pairs. To do so, we computed the similarity of neighboring axes using the Euclidean distance and used the maximal variance of similarities (MaxVar) as an objective function (see example in Figure 4). In summary:

| 3 levels of clutter (ON, 150N, 300N) × 31 participants | = 93 trials in total |

Post-processing. We collected the time to identify the number of clusters along with the similarity value of the selected axes pair. For comparison across datasets, we applied a linear min-max normalization to the similarity values of all neighboring axes pairs within each
better and more confident. We wanted to find out if participants are
informative about their preferences for a particular reordering.

4.4.2. Task 2 (Cluster Identification and Selection)
We wanted to find out if participants have better and more confident
preferences for a particular reordering strategy. In each trial, we presented
the participant one PCP, which was sorted by either SIM or DIS. The
participant had to select all clusters by choosing a pair of neighboring
axes and marking every cluster in both axes using a brush feature
(Figure 3 right). Brushing is applied by pressing the mouse button
and marking the cluster along the axis. The selection can be moved,
resized, or deleted. We do not highlight any data lines during or after
brushing. After confirming their selections, participants rated their
confidence in a correct clustering on a 5-point Likert scale.

Randomization. We selected 12 synthetic base datasets, three for
each number of clusters, and randomized the order. Then, we dis-
tributed the datasets into three equal-sized groups: ON, 150N, and
300N. Finally, we added four randomly selected real-world datasets
in a new group RW. Within each group, we randomly applied twice a
SIM and twice a DIS ordering. Participants worked on each group
in order of increasing difficulty (i.e., cluster level). In summary:

| Levels of clutter (ON, 150N, 300N, RW) | × |
| 2 repetitions | × |
| 2 ordering strategies (SIM, DIS) | × |
| 31 participants | = |

496 trials in total

Post-processing. We collected the time to mark the clusters and
divided this by the number of clusters to be comparable across
datasets. We also collected the selections and confidence levels.

We ignored clutter for the quality computation. We checked
whether participants selected clusters in two neighboring dimen-
sions and whether the number of clusters is therein consistent. In
132 trials, this was not the case, and we removed them from the
data. The results are, however, still trustworthy as the removed tri-
als are not skewed towards a particular reordering (66 trials each)
or a clutter level (32, 28, 28, and 44 trials). For all correct trials,
we then mapped the clusters between the selected axes together.
First, we compute the Overlap coefficient [Szy34] between all clus-
ter combinations and then merge the clusters with the highest over-
lap together. For each cluster combination, we keep the intersected
set of data records as cluster members. The Overlap coefficient
measures the overlap of members of the two clusters $C_i$ and $C_j$:

$$\text{overlap}(C_i, C_j) = \frac{|C_i \cap C_j|}{\min(|C_i|, |C_j|)}.$$ 

The quality of an entire clustering is based on the Jaccard index
[Jac01] between each selected cluster $C_i$ and the corresponding
ground truth cluster $G_i$. The Jaccard index measures the similarity
between the clusters (record sets) $C_i$ and $G_i$ on a data record level:

$$jaccard(C_i, G_i) = \frac{|C_i \cap G_i|}{|C_i \cup G_i|}.$$ 

As participants can also select too few or too many clusters, our quality computation is a two-
step process: First, we compute the average Jaccard index of each
cluster to their best match in the ground truth. Second, we compute
the average Jaccard index of every ground truth cluster to their best
match of our selection. Our final clustering quality is then the aver-
age score of both steps.

4.4.3. Task 3 (Ordering Strategy Preferences)
We wanted to find out if participants have preferences for a particu-
lar reordering and why this is the case. We presented them two PCPs
with the same dataset next to each other – one with SIM, one with
DIS ordering. Using two radio buttons, participants had to select
the preferred plot and then explain their choice in a free-text field.

Randomization. We randomly picked two synthetic datasets with a
different number of clusters. In the first trial, we did not show any
clutter (ON); in the second, we used either 150N or 300N (equally
balanced across the participants). In the first trial, we used SIM
ordering in the left, and DIS ordering in the right plot. In the second
trial, we swapped the positions. In summary:

| Levels of clutter (ON, 150N V 300N) | × |
| 31 participants | = |

62 trials in total

Post-processing. We stored the preferred ordering and the text for
each trial. Four participants reported not to see any preference be-
the options in one of the trials. We removed these participants
from the statistical analysis, but report their choices in Section 5.3.

4.5. Participants and Procedure
Prior to the study, we conducted several pilot runs in order to deter-
mine appropriate clutter levels and the number of trials for each task.

Participants. To have participants with basic knowledge in informa-
tion visualization and parallel coordinates, we conducted our user
study during two lectures at the University of Konstanz, Germany.
Both courses teach foundations in information visualization, one
course for undergraduates, the other for graduates. The courses were
taught by the same lecturer (not the authors), who also introduced
and discussed the PCP technique two weeks prior to the study. We
recruited 31 participants (17 male, 13 female, 1 NA). Their ages
ranged from 19–31 years (median age 23). Each participant had fin-
ished high school, and 17 held a Bachelor’s degree. The academic
background was in the area of data analysis with 24 computer sci-
ence, and 7 social and economic data analysis students. All partici-
pants reported having normal or corrected to normal vision.
Training and Procedure. All participants had to fill out a data privacy form in which we describe the data collected during the study. The participants sat scattered across the room and were not able to talk to each other. One of the authors started the study with a 30-minute recap on PCPs and comparing its visual patterns with scatter plots, discussing the advantages and disadvantages of the two techniques, and arguing about the effects of clutter, noise, and outliers. During the training, we did not provide strategies on how to identify clusters (or any other pattern) in PCP. Instead, we showed patterns in scatter plots and let all participants draw the respective patterns in a PCP (see training material). After this recap, we started the training. All participants opened their laptops and used a browser of their choice to access our online study. We provided a training platform, including all three tasks, but only two trials per task. We explained to the participants how to interact with the tool, and let the participants play around with the different trials. After answering the remaining questions, we made sure that all participants activated the full-screen mode within their browser and checked that the entire study could be conducted without scrolling for the different tasks. Participants needed between 20–30 minutes to complete the study.

5. User Study Results

We now report the summary statistics and highlight significant results ($p < .05$) in the data. For all tests, we checked the necessary preconditions, which can be found in the supplementary material along with the R scripts to reproduce the results. We used a one-sample Kolmogorov-Smirnov test to check if the data follows a normal distribution and Mauchly’s test to check for sphericity.

5.1. Task 1 (Similarity of Axes-Pairs)

We used a repeated-measures ANOVA for the analysis of completion time. The post hoc analysis was done with a Bonferroni corrected $t$-test for dependent samples. As the similarity of axes-pairs was not normally distributed, a non-parametric Friedman’s test was used.

Efficiency to Identify the Number of Clusters

There was a significant effect of clutter on completion time ($F(2, 60) = 6.07, p < .01, \eta^2 = .10$). Post hoc comparisons revealed that completion time was significantly lower for the clutter condition ON ($\mu = 9.44\)s) compared to 150N ($p < .01, \mu = 16.67\)s), and 300N ($p < .01, \mu = 17.47\)s), but not between 150N and 300N ($p = 1.0$).

Similarity of Selected Axes-Pair

No significant results can be reported ($\chi^2(2) = 4.77, p = .09$). As shown in Figure 5, the mean of the distances for the different clutter conditions were ON ($\mu = .53$), 150N (.71), and 300N (.75).

5.2. Task 2 (Cluster Identification and Selection)

For the comparison between clutter levels (independent of the ordering), we used a Kruskal-Wallis test and a Bonferroni corrected Wilcoxon signed-rank test for post hoc analysis. For the confidence, we applied a Pearson’s Chi-square test. To analyze the differences between the ordering strategies within each clutter level, we used a Wilcoxon signed-rank test for the analysis of completion time, cluster quality, and confidence. Data were split according to levels of clutter to compare the differences between SIM and DIS.

Efficiency to Identify and Mark Clusters

Between clutter levels, the medians of completion time for ON, 150N, 300N, and RW were 10.79, 9.53, 10.26, and 15.02, respectively. A Kruskal-Wallis test showed a significant effect on completion level ($\chi^2(3) = 23.31, p < .001$). A post hoc test using Wilcoxon signed-rank tests showed only significant differences between RW and ON, 150N, and 300N (all $p < .01$).

As shown in Figure 6, the medians of the completion time for the ON clutter condition, for SIM and DIS were 8.9s and 12.35s, respectively. A Wilcoxon signed-rank test showed that there was a significant effect of ordering strategy ($W = 1, Z = -2.46, p < .05, r = .25$). For the other clutter conditions, no significant results can be reported. For the 150N clutter condition, the medians of completion time for SIM and DIS were 10.67s and 8.58s, respectively ($p < .05$), for the 300N clutter condition, the medians of completion time for SIM and DIS were 11.12s and 9.62s, respectively ($p = .05$), and for the RW condition, the medians of completion time for SIM and DIS were 15.07s and 14.79s, respectively ($p = .82$).

Quality of Identified and Marked Clusters

Between clutter levels, the medians of quality for ON, 150N, 300N, and RW were .98, .91, .85 and .37, respectively. A Kruskal-Wallis test showed a significant effect on quality level ($\chi^2(3) = 181.56, p < .001$). A post hoc test using Wilcoxon Sign-rank tests showed the significant differences between ON and 150N ($p < .001$), 300N ($p < .001$), and RW ($p < .001$). Also, there were significant effects between 150N and 300N ($p < .05$), and RW ($p < .001$). Finally, 300N and RW were also significantly different ($p < .001$).

The results of the cluster quality are summarized in Figure 7. For the 150N clutter condition, the medians of quality for SIM and DIS were .87 and .94, respectively. A Wilcoxon signed-rank test showed a significant effect of ordering strategy ($W = 1, Z = -2.62, p < .001, r = .27$). For the 300N clutter condition, the medians of
We discuss the participants’ performance according to our hypotheses and highlight findings from the qualitative feedback of task 3.

### Influence of Clutter (H1)
Increasing the amount of clutter has a negative effect on the quality of the cluster identification and confidence of participants. These findings confirm H1 (b) and (c). While we see an increasing completion time for higher clutter levels in task 1, we cannot verify this finding in the second task. Hence, we cannot make a final judgment on H1 (a). As expected, clutter negatively influences the cluster identification. Patterns may vanish due to overlapping data lines, making the identification more difficult. Therefore, visualization experts need to carefully design PCPs and reduce the amount of clutter if possible (e.g., sampling).

### Reordering for Clutter-free Datasets (H2)
Similarity-based ordering strategies are a good choice for datasets without clutter. Our results show that participants perform the identification of clusters more efficiently when working with a SIM layout, which confirms H2 (a). It seems as if participants are faster in combining straight data lines into clusters in contrast to data lines with strong slopes. A possible explanation could be the Gestalt law [Wer23, War20] of continuation, which could help participants in tracking data lines across dimensions. Killman and Shipley [KSS91] support this argument: the angular parameters, determining the grouping of lines to clusters, may support the ability to find clusters across multiple sets of axes. The qualitative feedback also confirms our findings. Participants reported, for example, that “The structure of clusters is clearer”, “[clusters] don’t cross very often”, or they prefer SIM “[... since they do not intersect with each other in the majority of areas between each two dimensions [...]”. We cannot support hypotheses H2 (b) and (e). There are no significant differences in the cluster identification quality or the confidence of the participants (see also Figure 7 and 9). Also, participants did not have a subjective preference for a particular reordering strategy, as shown in Figure 8.

### Reordering for Cluttered Datasets (H3)
For datasets with clutter, there is strong evidence that DIS layout strategies are more suitable. The quality of marked clusters is significantly better when participants used a DIS ordering strategy, confirming H3 (b). This finding coincides with the reported confidence of participants (see Figure 9), who are also significantly more confident when working with DIS in clutter conditions. Even if both options are available (SIM and DIS), there is statistical proof that participants will choose a DIS ordering in clutter conditions providing evidence for H3 (c).

The Gestalt law of grouping by orientation similarly [Wer23, War20] might be a reason for this preference. The orientation of the lines is more salient in the DIS ordering, which facilitates a stronger grouping compared to a SIM ordering.

We cannot see significant differences in the similarity values of...
Whenever possible, clutter should be removed in a pre-processing step. Results from tasks 1 and 2 indicate that participants working with PCPs need more time, are less accurate, and are less confident in identifying clusters with an increasing amount of clutter.

For datasets without any clutter, a SIM layout should be preferred over a DIS layout. Participants working with a SIM ordering strategy were faster in identifying and marking clusters compared to a DIS layout, as results indicate in task 2. There is, however, no difference in the quality of the clustering or confidence.

When clutter is an issue, a DIS ordering strategy should be preferred over a SIM layout. As we can see in the results from tasks 2 and 3, participants performed more accurately and were more confident in their selection when working with a DIS layout.

Although we used two clutter conditions in our study, it is challenging to derive specific guidelines when a dataset is considered cluttered. It depends on many properties, such as the number of records, the general density of data and patterns, and the size of the PCP. Therefore, this needs to be analyzed in follow-up studies.

6.2. Limitations and Future Work

In our study, we focused on cluster identification. Therefore, the proposed design considerations need to be considered with caution for other tasks like correlation analysis. There might be changes in performance due to different patterns of interest. The same is true for the cluster structures. Our synthetic benchmark consists of a strong cluster structure throughout all dimensions. The results of our study might not be representative if cluster structures are less compact or not present across all dimensions. The results of our study already show that real-world datasets perform significantly worse than the synthetic benchmark data, although we selected datasets, commonly used in PCP research. The reasons for this effect might be that (1) all records of the real-world data belong to a cluster (no clutter was present), (2) the clusters in the real-world dataset were less compact than in the synthetic datasets, and (3) the real-world trials were done right after the 300N trials. Hence, participants selected only a subset to be part of a cluster and interpreting the remaining points as clutter. To generalize our results further, a follow-up study with different datasets should be conducted.

Further limitations of the study are (1) The number of dimensions and records: while we believe that results are independent of the number of dimensions, we restricted ourselves to eight dimensions to keep the trials throughout the study comparable. With an increasing number of dimensions, the computation of ordering algorithms will take longer; however, this was out of the scope for our study to investigate. (2) The population of participants: The study was conducted during two InfoVis lectures at our university. Therefore, participants were recruited from an InfoVis-trained, local student population, limiting the generalizability of the results. (3) Study setup: Participants used their own laptops with different screen space and resolution. Although we manually checked that the study was displayed correctly on each laptop, the experience might change due to different screen settings or selected internet browser.

7. Conclusion

This paper advances the field of axes reordering in parallel coordinates plots (PCPs). First, we classified existing reordering techniques based on their inner workings, preferred patterns, and meta characteristics. Using this classification, we provide guidance in selecting an appropriate approach for a given task. Second, we pushed the evaluation of axes reordering techniques towards empirical justification. We conducted the first controlled user study to assess the performance of PCPs with two different ordering strategies. Specifically, we investigated whether the often proposed similarity-based axes arrangement (SIM) is better to identify clusters than a dissimilarity-based layout (DIS), which produces more salient cluster patterns. Our results show that, depending on the clutter level, participants performed differently based on the used ordering strategy. When no clutter was present, a SIM layout was more efficient, whereas, for cluttered datasets, a DIS layout led to better results. The subjective preference of participants supported these findings. Thus, our study shows that the performance of participants can be increased by choosing the correct layout strategy based on the underlying task.

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