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Visualizing Dimensionality Reduction Artifacts: An Evaluation

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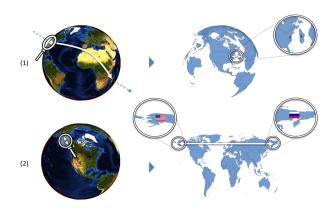


Figure 1: Multidimensional projection artifacts are identical to geographic projections artifacts when we project the Earth on a 2D plane: (1) The orthogonal projection exhibits false neighborhoods: here, Washington appears right next to Antananarivo. (2) The Mercator projection exhibits tears: the Earth has been unfolded along the equator, leading to display Alaska far away from Russia. These artifacts always exist when projecting high-dimensional data with any dimensionality reduction technique.

Abstract

Multidimensional scaling allows visualizing high-dimensional data as 2D maps with the premise that insights in 2D reveal valid information in high-dimensions, but the resulting projections always suffer from artifacts such as false neighborhoods and tears. These artifacts can be revealed by interactively coloring the projection according to the original dissimilarities relative to a reference item. However, it is not clear if conveying these dissimilarities using color and displaying only local information really helps to overcome the projections artifacts. We conducted a controlled experiment to investigate the relevance of this interactive technique using several datasets. We compared the bare projection with the interactive coloring of the original dissimilarities on different visual analysis tasks involving outliers and clusters. Results indicate that the interactive coloring is effective for local tasks as it is robust to projection artifacts whereas using the bare projection alone is error prone.

Categories and Subject Descriptors (according to ACM CCS): Information Interfaces and Presentation [H.5.2]: User Interfaces—Evaluation/methodology

1. Introduction

Multidimensional data is ubiquitous: all domains including sciences and engineering need to analyze and make sense of it. Several visualization techniques are known to be effective for data up to 10-15 dimensions, such as scatterplot matrices [CM88] and parallel coordinates [Ins85], but they become unusable when the number of dimensions grows. Data then becomes high-dimensional and fewer techniques are effective. Multidimensional scaling is one of them: it tackles the visualization problem by summarizing many dimensions into a similarity matrix that is visualized as a 2D scatterplot called a *projection*: 2D distances between points in the projection are meant to preserve the original dissimilarities between data items in high-dimensions.

Projections have been mainly applied in domains where users are data scientists who want to get insights about their high-dimensional data [BSIM14]. However, the most promising applications might be in domains where users are not professional analysts but need to make decisions about high-dimensional data. The assumption being that if visual patterns visible in 2D reveal patterns in high-dimensions, then with only a short training, anyone should be able to detect these patterns.

A large number of projection algorithms [vdMPvdH08] have been designed to effectively and efficiently map a set of data items from a high-dimensional space (*data-space*) to a lower dimensional space (*2D-space*), while preserving as much information as possible. However, as good as these algorithms can be, the dimensionality reduction process necessarily implies a loss of information that is materialized by distortions such as topological artifacts (Figure 1). These artifacts interfere with the visual analysis process and challenge the *interpretation* and *trust* [CRMH12] of projections.

Some existing measures quantify and can reveal artifacts, *e. g.* through coloring problematic points [MCMT14]; they can also help choosing relevant projections through visual quality criteria [BTK11]. However, these existing approaches provide hints on possible artifacts but do not actually help overcome them for analyzing data clustering.

Aupetit introduced a technique in [Aup07] that colors projections according to the original dissimilarities relative to a reference item interactively selected by a pointer. This technique not only reveals artifacts but additionally shows information about the data-space through the color channel. However, it is not clear if visualizing dissimilarities through the color channel is effective to perform important tasks such as detection of clusters and outliers.

The background section describes the challenges of assessing projections quality and explain how projection artifacts impact visual analysis tasks based on projections. We then introduce our method to visualize artifacts, and describe our experiment design and its results before concluding.

2. Background

This section presents approaches that assess projections quality and tend to take projection artifacts into account. To our knowledge, there is no controlled experiment to report on the effect of these artifacts and their counter measures but we still report on evaluations related to projections.

2.1. Projections Quality

Arguably, artifacts could be avoided or become negligible if the projection quality were good enough. Different approaches exist in the literature to assess the quality of a dimensionality reduction process [FSJ13]. Because projection algorithms are black-boxes, these approaches tend to help choosing and setting an algorithm that will provide a projection that can be easily and faithfully interpreted. We can distinguish approaches that target an automatic processing of dimensionality reduction [BTK11] and other interactive approaches that provide measures and visualizations to help users explore different projection settings, such as the Dim-Stiller system [IMI*10]. Both approaches have to define first how to measure the quality of projections, and understanding the measures is far from simple.

The quality of projections can be defined through particular visual criteria such as "outlying", "clumpy", "skinny" [WAG05]; it can also rely on task completion time benchmarks, such as visual clustering [BTK11]. There are many ways to define and evaluate visual clustering such as class consistency, cluster separation [SNLH09] or class density [TBB*10]. However these automated measures still do not compete with human judgment as it is hard to summarize visual complexity and it is very dependent on data characteristics. Moreover measures such as cluster separation were proved as not reliable to judge the quality of a projection [STMT12].

A good projection mapping can be defined as one that minimizes the *projection stress* [Tor52], *i. e.* the least squares error between distances in data-space and Euclidean distances in 2D space. The closer the distances are, the lower the stress is. However, each projection algorithm, and especially multidimensional scaling projections, gives its own stress definition through the objective function it optimize. Once a stress measure is defined, it can be visualized either statically or interactively.

A common technique maps the stress measure optimized by the algorithm using a visual variable on each dots; usually, each dot is colored depending on its stress value using a color scale from yellow (low stress) to red (high stress) [BW96]. Other visual encoding techniques exist to display the stress measures such as *jitter disc* [BCLC97], or *interpolated coloring* [SvLB10]. However, visualizing the stress alone only warns users about potential issues with the position of the points, but they do not provide any hint on the nature of these issues.

2.2. Projection artifacts

Even if projection algorithms tend to preserve "most of" the important aspects of the underlying data structures existing in data-space, all the 2D distances do not faithfully respect data-space distances: some points are misplaced and we call these points *artifacts*. We distinguish geometric artifacts [Aup07] from topological artifacts [LA11].

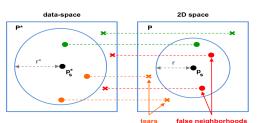


Figure 2: Model characterizing the different types of points relative to the reference point (in black). The neighborhood of the reference in the data-space is represented by a sphere of radius r^* centered in the reference p_s^* . And in the same way, its neighborhood in the 2D space is represented by a disc of radius r centered in p_s . Points in the neighborhood of the reference are represented by a circle and the other by a cross. The points are either topological artifacts, i. e. false neighborhoods (in red) and tears (in orange), or well placed points (in green).

Geometric artifacts are caused by small distortions of distances such as compressions and stretching. The perceived 2D distances are inaccurate but neighborhoods are preserved: these artifacts do not impact directly interpretation trustworthiness as clusters are neither split nor merged. When distortions are "important", they can lead to topological artifacts: the visible neighborhood is wrong, some items seem close when they are actually far-away in data-space (false neighbors) while items that are close in data-space become far-away in 2D-space (tears). These artifacts are more problematic for analysis tasks: they distort 2D clustering and lead to misinterpretation.

Topological artifacts involve two important aspects: first, they are *relative* to a reference item or cluster. For example, a point that is a false neighbor for its 2D neighbors may also be a tear for its data-space neighbors (Figure 2). Second, topological artifacts have different levels of granularity. The definition of these artifacts relative to a reference item transfers relative to a reference cluster. Two distinct clusters in data-space may be projected in the same area on the projection and then become false neighbors. In the same way, one cluster in data-space can be split into disconnected components in 2D space, and each component is a tear relative to the other. Splitting clusters "only" impacts interpretation trustworthiness made from the projection, but false neighbors also impact the visual quality of the projection by deteriorating the visual separability of clusters. These artifacts damage the interpretability of projections at different levels depending on the considered visual analysis task.

Recently, Martins et al. [MCMT14] proposed a system with different views, each one indicating either the global stress, or false neighbors or tears according to different scales (relative to an item or a cluster). Different measures are proposed for each type of artifacts and are represented on each view using color interpolation or bundled edges linking the original neighbors on the projection to highlight tears. These edges are colored according to the error intensity. To control the clutter of the edges, user can select a point or a set of points to focus the visualization around their relative topological artifacts. This system helps understand the impact of the parameters and algorithm choices on the projection quality, but it does not directly help to reveal actual clusters hidden by projection artifacts.

Using a uniform color scale, the *proximity-based visualization* [Aup07] corresponds to the interactive coloring of projections based on the original dissimilarities, that we presented in Figure 3. This technique displays interactively at each point its original dissimilarity in the data-space relative to a reference data item selected by the user on the projection. Distortions are indirectly visualized by contrast between 2D positions and colors representing the original dissimilarities. This technique may address visual analysis tasks such as validating outliers or visual clustering, but it displays local information relative to a reference item and its visual encoding needs to be validated. In this paper we report on a controlled experiment with the aim of evaluating the effectiveness of this technique compared to the bare projection with regard to different visual analysis tasks.

2.3. Projections Evaluation

Several kinds of studies exist to compare the performances of projection algorithms [BJD81]. These studies consider a quality metric and a predefined setup of parameters to compare the algorithms on benchmark data sets. However, these studies do not address the human ability to interpret the results of the algorithms.

Few user studies have been done on how the visualized projection are interpreted [IR11]. Recently, an evaluation on how experts and novices judge the quality of projections has been published [JML12], showing that experts are consistent in their analysis where novices are more random. The visual encoding of the projection as a 2D, 3D or SPLOM scatterplot has also been studied [SMT13] and shows that the 2D scatterplot used with SPLOM really helps user perform exploratory analysis with projections.

3. Assessing the Impact of Projection Artifacts

In this article, we want to assess how projection artifacts impact the interpretation of multidimensional scaling techniques, and in particular if we can overcome these artifacts using a —preferably simple— technique.

The *proximity-based visualization* [Aup07] is a simple technique; unlike other techniques it does not require any parameter, only the user selection of a reference point. The

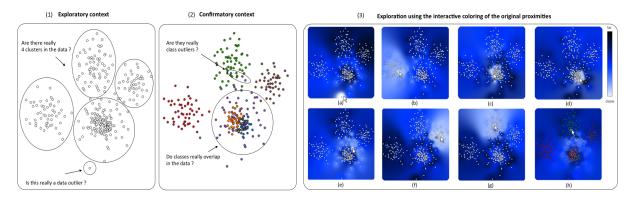


Figure 3: Main questions involved by the visual analysis of projections in exploratory and confirmatory contexts (1,2). Exploring the projection with the interactive coloring of the original dissimilarities gives an answer to each question (3). Indeed, the gaps in the projection colorings (from white to blue) show that there are six underlying clusters in the data (b,c,e,f,g,h). We also observe that the point at the bottom of the projection (1) seems to be actually a data outlier (a) and that the three points at the top of the projection (2) are not actually class outliers (h). The projection was obtained from the PCA of a synthetic dataset composed of 6 clusters generated from Gaussian distributions randomly centered in a 10-dimensional space. The reference point of the interactive coloring is the point with the whitest color, and is also the closest point from the mouse cursor. The whiter the color, the lower the dissimilarity to the reference in the data-space.

idea is to convey proximities in data-space using color in addition to their spatial encoding. Displayed dissimilarities are relative to a reference item that implies exploring interactively the projection using a pointer. As this technique displays original information in addition to the projection mapping, it can help dealing with projection artifacts and help building a more reliable mental model of the proximity relationships in data-space.

However it is not clear if visualizing the dissimilarities using color is effective to help performing visual analysis tasks on projections that present artifacts. Therefore, we designed a controlled experiment in order to assess the potential of this technique. With this experiment, we address the following research questions:

- 1. Can we help non specialists deal with visual analysis tasks using projections, independently of the inherent quality of these projections?
- 2. How do artifacts impact the visual analysis of projections?
- 3. Is the interactivity required by proximity-based visualization worth its improvements in accuracy?

In the following, we refer the bare projection simply as *Projection* and the *proximity-based visualization* [Aup07] as *ProxiViz.* We first describe the tasks, techniques and datasets we consider in the experiment before presenting how we assess projection quality for each task. We then introduce the experiment procedure and participants before presenting our hypotheses and the experiment results.

3.1. Tasks

Recently, a characterization of task sequences for the visualization of dimensionality-reduced data has been established from interviews with data analysts [BSIM14]. In this article, we consider multidimensional scaling techniques, therefore we focus only on cluster-oriented task sequences. Among the three task sequences proposed, we consider only the sequences "verify clusters" and "match clusters and classes", as the sequence "name clusters" would require participants to have prior knowledge in data. We define data outliers as particular cases of clusters: they are composed of only one data item; And class outliers are defined as mislabeled data items. We considered the following tasks and questions:

Data outlier validation: for a highlighted dot on the projection, participants have to choose a yes/no answer to the question "Is this a data outlier?".

Clustering validation: for two differently colored sets of highlighted dots on the projection, participants have to choose a yes/no answer to the question "Do these two sets of points belong to the same cluster?".

Clusters enumeration: participants have to answer the question "How many clusters can you count?" looking at the projection. They are allowed to answer 1 to 7.

Class outliers validation: for a highlighted dot on the class colored projection, participants have to choose a yes/no answer to the question "Is this a class outlier?".

3.2. Techniques

We used the two following techniques:

Projection is static and displays a dot for each point with

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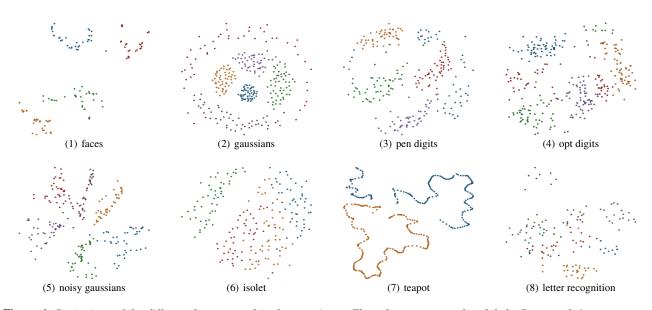


Figure 4: Projections of the different datasets used in the experiment. The colors represent class labels. Datasets 1-4 were considered as easy for a visual clustering task and datasets 5-8 were considered more difficult to analyze as the 2D clusters are less separated. Labels were indicated only for the class outliers validation task.

no color encoding. This visualization corresponds to a spatial encoding of the dissimilarity matrix. 2D distances between points tend to respect the original dissimilarities between data items.

ProxiViz is interactive and displays colors representing the original dissimilarities relative to a reference point. This interactive technique is a color encoding of only one row of the dissimilarity matrix. When the mouse moves over the visualization area, the nearest point is interactively selected as *reference* [Aup07]; the color encoding of the visualization is immediately updated to display dissimilarities to the reference in the data-space. We use a uniform shade of blue colorscale that vary in intensity to color the proximities (*i. e.* inverse *dissimilarities*). It starts with a white color indicating close-by items (*i. e.* with a null dissimilarity), then continues with blue nuances, and ends with black, indicating the farest items with maximum dissimilarity to the reference.

The original *proximity-based visualization* uses color to encode dissimilarities and it applies color on the Voronoi cell of each point. However the size of the Voronoi cells depends on the density of points and may vary arbitrary across the projection, which can introduce biases as this size does not encode any information.

We performed a pilot experiment with both synthetic and real datasets to choose a good visual encoding for ProxiViz. We compared applying coloring to points, to Voronoi cells and to background using color interpolation based on the inverse-distance weighting. This interpolation used with ProxiViz displays the global proximity trends in each area of

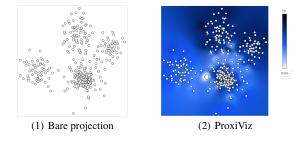


Figure 5: Projection and ProxiViz as used in the experiment. The colorscale was shown to help analyzing the coloring. The gaps between colors intensity on the projection indicate gaps of dissimilarities in the data-space.

the projection while preserving the local proximity information with a shaded circle around each point (Figure 5).

For a cluster enumeration task, the results of the pilot show that ProxiViz with the color interpolation was significantly more accurate that the other color encodings and overall preferred by the participants for its precision and aesthetic. We implemented the projection visualization in d3.js [BOH11] and the color interpolation using WebGL Shaders. This implementation scales up to one thousand items, so the interaction was fluid with our datasets.

5

Name	Dimensions	Instances	Clusters	MDS
gaussians	100	300	6	NerV
noisy gaussians	100	240	6	NerV
pen-digits	16	250	5	classical
opt-digits	64	300	6	NerV
isolet	617	200	4	classical
letters	16	180	6	classical
faces	960	128	4	NerV
teapot	192	365	2	NerV

Figure 6: Summary of the characteristics of each dataset used in the experiment.

3.3. Datasets

We used high dimensional datasets and made sure that the ground truth (corresponding to class labels) was verified by the dissimilarity measure. More precisely, we verified that for the dissimilarities in the data-space, one cluster exists for each class label and that this cluster does not overlap with other clusters. We chose only datasets for which this criterion was verified. We then projected datasets using two different projection algorithms: classical MDS [Tor52], erV [VPN*10], using different settings of the parameters. We visually checked the clusters separability and selected the projections to balance questions difficulties.

Real datasets were mainly taken from [FA10]: Pen-Based Recognition of Handwritten Digits (*pen-digits*), Optical Recognition of Handwritten Digits (*opt-digits*), Isolated Letter Speech Recognition (*isolet*), Letter Recognition Dataset (*letters*), CMU Face Images Dataset (*faces*) and Teapot Dataset (*teapot*) from [ZL05]. We also generated two synthetic datasets with clusters based on Gaussian distributions with random noise applied to some features of the second dataset (*gaussians* and *noisy gaussians*).

In order to justify the use of multidimensional scaling instead of linear projections, we favored datasets from image and signal processing as their dimensions were not directly interpretable. The two synthetical datasets helped to balance questions difficulties. More details are provided in Figure 6.

3.4. Difficulty

We visually explored each projection and detected local artifacts. Then we set the questions and their answers manually for each task and dataset in order to balance the questions in two categories: easy and difficult. Easy questions are questions that can be answered with no additional information and difficult ones involve topological artifacts or cluster separation problems.

We used visual exploration and automated algorithm to suggest clusters and possible outliers using the scikit-learn library [PVG*11]. We then selected interesting cases balancing the questions difficulties:

Data outlier validation: we had to find data outliers for each dataset. Using One Class SVM [SWS*99] and Local

Outlier Factor [BKNS00], we selected two sets of data outliers. We visually selected one outlier at the intersection of the two sets. An easy question is when the outlier is well separated from the closest blob of points whereas a difficult one is when it is not.

Clustering validation: we had to select different clusters and cluster components for each dataset. We visually selected two sets of points close in 2D space and we analyzed their connections using the k-nearest neighbors. Difficult questions involve either tears or false neighborhoods. **Clusters validation:** we had to analyze the quality of clustering of each dataset. We verified the ground truth corresponding to labels by checking that each class had an underlying cluster and that clusters did not overlap too much each other. We then categorized the questions depending on how clusters were visually separated on the projection.

Class outlier validation: we had to extract class outliers for each dataset. Using KNN Classifier [CH06] and One Class SVM [SWS*99] on each class, we visually determined an interesting class outlier for each dataset. Difficult questions involve either tears or false neighborhoods.

We tried to avoid questions that would be too easy or too hard to answer either with Projection or ProxiViz. We expected that ProxiViz would be more accurate than Projection on difficult questions and that the techniques would be equally accurate on easy questions.

3.5. Experiment design

We used a within-subjects design with no repeated measures and the following factors: Technique and Difficulty. The order of blocks and trials were counterbalanced using a Latin Square. We also changed the orientation and flipped the display along one axis between each block for each projection. Each participant faced successively 2 blocks (one for each technique) of 24 trials (3 tasks \times 8 projections) and then 2 blocks for the class outliers validation task with 8 trials each.

We kept the blocks order with Projection first, because ProxiViz displays more information and users would be biased when revisiting the same projection using the bare condition. Indeed, during the pilot session, we observed that participants recognized datasets when using ProxiViz before Projection and not when using Projection first. Introducing this order for the techniques may slightly bias our results, but we believe that considering our high level tasks, it is important to avoid the observed learning effect while keeping the conditions equivalent by reusing the same projections.

In summary, the design included:

1,536	trials in total	
24	participants	=
64	trials per participants	×
2	techniques (blocks)	=
4	tasks	\times
2	difficulties	×
4	projections	\times
-	-	

3.6. Participants

The participants of our experiment are data analysts who aim at understanding underlying data structures in highdimensional data, *i. e.* outliers or clusters. These data analysts can be domain experts, statisticians, or data miners; they know how to interpret projections resulting from dimensionality reduction and we made sure they were aware of their possible artifacts.

24 participants (8 women and 16 men) from 23 to 37 years old (avg. 28) from two laboratories specialized in data analysis completed the evaluation. They all had a computer science background but in different domains: statistics, signal processing, image processing, machine learning, data mining. Their application fields were also varied in the same way that their level of expertise regarding data analysis. They rarely looked at projections but they had knowledge about projections techniques overall. They were used to static visualizations such as those available in different statistical analysis software (matlab, R). They all had a normal vision with no color vision problems.

We did not consider recruiting novice analysts as it would have required training them to understand dimensionality reduction and perform visual analysis of projections; still, our participants were not experts in multidimensional scaling.

3.7. Procedure

We recorded the answer and response time of each participant for each question. Participants used only the mouse to interact with the system and answered questions by selecting a row in a multiple-choice form (yes/no or 1 to 7 clusters). Timing was started once a technique appeared on the screen and stopped when the participant validated the answer. After each validation, we also asked the confidence level regarding the answer (five-points Likert scale). Between each block, the participants were free to rest a bit. We imposed a duration of 30-60 seconds maximum for each trial, for a total evaluation duration of around 30 minutes, preceded by 20 minutes of presentation of the evaluation and a training. The evaluation system was run in a Chrome web-browser displayed in full-screen resolution 1440 \times 900 of a MacBook Pro display.

After a short introduction on artifacts and visual analysis, we verified that the analysts understood the techniques and agreed with our definitions of data outlier, cluster and class outlier. We trained subjects on a simple dataset for each technique and task, and we let them explain their reasoning for each answer. If necessary, we explained the pitfalls of their reasoning and how they should understand the problem.

We used 6 subjects for a pilot to update the procedure of the experiment and verify results consistency. Before the study, participants filled a questionnaire eliciting demographic information and to check for possible color blindness. After the study, participants also filled a questionnaire of subjective preferences for the different techniques to collect feedback on their user experience.

3.8. Hypotheses

Our hypotheses are that ProxiViz will be more accurate than Projection overall, and even more so on difficult questions, both for local tasks involving outliers or clusters, and visual clustering tasks implying to explore the whole projection. We also hypothesize that participants will be significantly slower using the ProxiViz technique. However we do not expect significant differences on easy questions for each task between ProxiViz and Projection.

Based on our experience and our three research questions introduced previously, our hypotheses were as follow:

- **H1** For each task, we expect that ProxiViz is more effective than Projection in terms of accuracy.
- **H2** For each task, we expect ProxiViz to be more effective than Projection for difficult questions and as effective as Projection for easy questions.
- **H3** For each task, we expect that participants will be significantly faster using Projection.

4. Results

We transformed the error into a percentage of correctness: for tasks that expect a yes/no response, the correctness is either 100% or 0% if the answer is right or wrong. For clusters enumeration, the error is calculated as the difference between the number of clusters found c and the number of clusters really present in the data c^* . We use in the sequel a percentage of correctness v based on this formula:

$$v = \begin{cases} \left| \frac{c - c^*}{8 - c^*} \right| \times 100, \text{ if } c > c^* \\ \left| \frac{c - c^*}{1 - c^*} \right| \times 100, \text{ if } c \le c^* \end{cases}$$
(1)

Since our design is within-subject with repeated measures and that correctness do not follow a normal distribution for all tasks, we used Friedman's test for one way analysis of variance to analyze more than two non-parametric distributions, and pairwise Wilcoxon signed rank test with Bonferroni correction to analyze two independent non-parametric distributions. We log-transformed the response time to better fit a normal distribution and verified this assumption using a Shapiro-Wilk test (p > .05). We then used the one-way repeated measure ANOVA and paired t-tests to analyze response time.

In terms of correctness, Friedman's test reveals a significant effect of the factor Technique for each task, except for clusters enumeration. A significant effect of both Technique and Difficulty was found for each task. Overall participants obtained more good answers using ProxiViz than Projection for each task except for clusters enumeration. The details are shown in Figure 7.

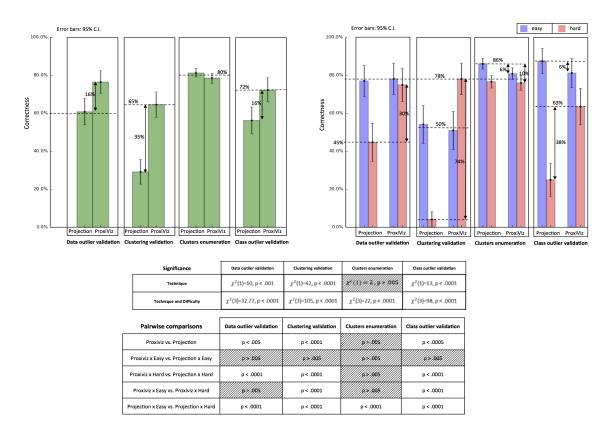


Figure 7: Results of average correctness (in %), significance between factors given by Friedman's test, and pairwise Wilcoxon signed rank test results.

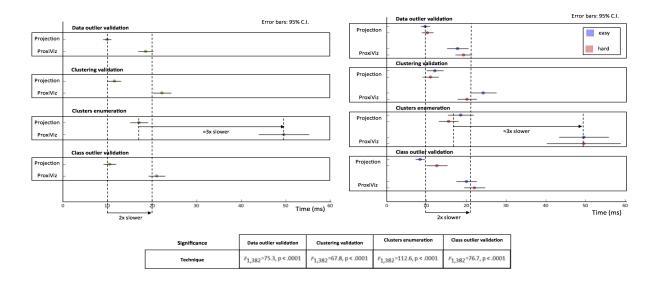


Figure 8: Results of average response time (in seconds) and significance between factors given by ANOVA.

In terms of response time, ANOVA reveals a significant effect of the factor Technique and no significant interaction between Technique and Difficulty. No significant differences were found in response time between easy and difficult questions for each pair of technique and task. Pairwise comparison of the two techniques revealed that ProxiViz is significantly around 2 times slower (p < .0001) than Projection for each task, except clusters enumeration for which ProxiViz is significantly 3 times slower (p < .0001) and both on easy and difficult questions. More details are shown in Figure 8.

4.1. Confidence and User Preferences

No significant differences were found for the confidence answers between the two techniques. For all tasks, users felt confident except for clusters enumeration where they were neither confident nor skeptical for both technique. Low correlations were found between confidence and correctness, and between confidence and time.

We used these confidence results to check that difficulty levels were well calibrated and that none of the questions were too difficult or too easy to answer from the participants' point of view. We would have expected that participants felt more confident using ProxiViz but it was not the case as they were not always able to interpret easily the coloring or to reconstruct the clustering using relative proximities gathered during exploration.

Overall ProxiViz was preferred to Projection (20 participants). 18 participants felt more confident and preferred ProxiViz for its clarity. 18 participants felt faster using Projection. 21 felt that they were making correct choices using ProxiViz and 16 were satisfied by their choices. Some participants said they felt responsible for the errors because they were not able to accurately decode the additional information provided by ProxiViz.

5. Discussion

In this section, we discuss the results regarding our hypotheses which are overall supported.

H1: For each task, we expect that ProxiViz is more effective than Projection in terms of accuracy.

For data and class outliers validation, **H1** is supported as overall, ProxiViz was significantly (16%) more accurate than Projection. For clustering validation also, ProxiViz is significantly (35%) more accurate than Projection. However, **H1** is partially supported because for clusters enumeration ProxiViz is not significantly more accurate than Projection.

This last result is not surprising as ProxiViz gives better insights on local information relative to one reference item. Generalizing each relative coloring to perform visual clustering requires to explore the whole projection with the pointer, relying on the human memory to reconstruct the clustering, which implies a high cognitive load. In particular, we noticed during the evaluation that participants felt lost on this task using ProxiViz as the dissimilarity distributions were really different from one dataset to the other. Some participants felt also lost during their exploration as colors changed dramatically when moving from one reference to another.

Moreover the difference of color intensities between clusters was sometimes difficult to assess to delimit clusters. In particular, we noticed that some participants used the 2D positions instead of the coloring when they considered that color difference was too difficult to interpret and the 2D distances good enough. This suggests that the bare projection gives a suitable overview of the data clustering.

Overall results show that participants were on average effective at analyzing the colors displayed by ProxiViz (60% to 80% accurate). ProxiViz is also significantly more reliable than Projection for outliers and clusters validation. So ProxiViz can help non-specialists deal with label matching tasks and tasks related to class structure in a confirmatory context, irrespective of the inherent quality of the projection considered. Note that we considered a dissimilarity matrix that reflected the class model, and we did not took into account the inherent problem of finding and validating such dissimilarity measure.

H2: For each task, we expect ProxiViz to be more effective than Projection for difficult questions and as effective as Projection for easy questions.

For data and class outliers validation, **H2** was supported as ProxiViz was 30-38% more accurate than Projection on difficult questions. For clustering validation also as ProxiViz was 74% more accurate than Projection on difficult questions. Furthermore, for class outlier validation, we observed that the 6% difference of correctness on easy questions between ProxiViz and Projection was significant.

For clustering validation, correctness results are very low for hard questions using Projection. For this task, artifacts involved in hard questions were almost impossible to detect using Projection. However using ProxiViz, they were revealed and participants were able to use their finding to answer questions without having to explore, which explains that correctess results were better for hard questions than for easy questions using ProxiViz.

We noticed during the evaluation that participants had sometimes problems to recall the definition of a class outlier and the question may have not been well expressed. For this task, participants had to verify that the highlighted point was not in the neighborhood of the other points of its class. So they had to verify that: "no, the point is not in the neighborhood of the class" to answer "yes, this is a class outlier". Using Projection, verifying the neighborhood is quickly done and some participants may have made mistakes because they answered too quickly, not following the right reasoning, which was clearly uneasy. For clusters enumeration, **H2** was partially supported, as ProxiViz was not less accurate than Projection on difficult questions. Nevertheless for clusters enumeration, we observed that the 6% difference of correctness on easy questions between Projection and ProxiViz was significant. This suggest that when clusters are well separated, Projection gives a better overview of the data clustering than ProxiViz.

Considering all tasks and techniques, we can notice that the highest correctness is close to 90% and the lowest correctness close to 5%. This suggests that questions were neither too easy nor too hard, and especially for local tasks that required a yes/no answer. These results might be improved using a longer training of participants to make them share the same visual criteria defining outliers and clusters.

Overall, our results show that ProxiViz is more robust to artifacts than Projection. For local tasks, analysts must clearly be explained the dangerous impact of artifacts. Conversely for more global tasks involving visual clustering, it seems that the impact of artifacts is less important. The static projection is a good tradeoff to obtain an overview of the data clustering. However we still need to evaluate if other techniques that enhance the projection may improve the accuracy of visual clustering.

H3: For each task, we expect that participants will be significantly faster using Projection

For data outliers, class outliers and clusters validation, H3 was supported, as overall ProxiViz was significantly slower (around 2 times) than Projection on both easy and difficult questions. For clusters enumeration, H3 was also supported, as overall, ProxiViz was significantly slower (around 3 times) than Projection on both easy and difficult questions. Overall no significant differences were found between easy and difficult questions for each technique and task.

Exploring projections for local tasks with ProxiViz does not require a large difference of time compared with Projection. Moreover this time is independent of artifacts. ProxiViz is then worthwhile to dig into the details, as users will feel more responsible for their choices because these choices are resulting from a methodical exploration instead of an overview for which we know artifacts happen.

6. Conclusion and Future Work

In this article, we have investigated how artifacts inherent to multidimensional projections interfere with the interpretation of these visualizations, and the effectiveness of the ProxiViz technique to facilitate the detection and interpretation of these artifacts. The ProxiViz technique interactively colors the whole visualization when the user moves the pointer to a particular point: it shows a color-map where the intensity decreases with the dissimilarity in data-space from the focus point, conveying dissimilarity information using the color channel. We conducted a controlled experiment to evaluate the effectiveness of ProxiViz compared to the bare projection with regard to different visual analysis tasks. These tasks require both local and global exploration, and involve both outliers and clusters detection.

Results show that ProxiViz is effective to perform local tasks such as label matching of outliers and clusters. Moreover this interactive technique is robust to the artifacts whereas the bare projection is not for the considered tasks. Conversely, for visual clustering tasks, results show that the impact of artifacts is less important and that projections give a suitable overview of the data clustering. The ProxiViz technique is therefore a valuable interactive enhancement for projection-based systems.

Projection-based visualizations have applications in domains where users are not analysts but need to make important decisions about high-dimensional data. One example is cargo scanning, used by customs to check the contents of freight shipping containers as quickly as possible. The scan of a container returns multidimensional information that needs to be checked against the list of goods declared to be in the container. This list of goods (*e. g.* toys, furniture) is translated into multidimensional information and projected over the scanned information. Some decision needs to be done about the container: let it go, fast check, or in-depth check. This decision can be critical and relies on human judgment to interpret the possible issues. Our results indicate that ProxiViz is suitable for this use case as is robust to projection artifacts for outlier detection.

As projection artifacts have still a significant effect on local analysis, measures and approaches that help assessing the quality of projection must be generalized in existing softwares that visualize high-dimensional data with projections.

References

- [Aup07] AUPETIT M.: Visualizing distortions and recovering topology in continuous projection techniques. *Neurocomputing* 70, 7-9 (2007), 1304–1330.
- [BCLC97] BRODBECK D., CHALMERS M., LUNZER A., COT-TURE P.: Domesticating bead: adapting an information visualization system to a financial institution. In *Proceedings of the 1997 IEEE Symposium on Information Visualization (InfoVis* '97) (1997).
- [BJD81] BISWAS G., JAIN A., DUBES R.: Evaluation of projection algorithms. *IEEE Transactions on Pattern Analysis and Machine Intelligence PAMI-3*, 6 (1981), 701–708.
- [BKNS00] BREUNIG M. M., KRIEGEL H.-P., NG R. T., SANDER J.: Lof: identifying density-based local outliers. In Proceedings of the 2000 ACM SIGMOD international conference on Management of data (2000), SIGMOD '00, pp. 93–104.
- [BOH11] BOSTOCK M., OGIEVETSKY V., HEER J.: D3: Datadriven documents. *IEEE Trans. Visualization & Comp. Graphics (Proc. InfoVis)* (2011). URL: http://vis.stanford. edu/papers/d3.
- [BSIM14] BREHMER M., SEDLMAIR M., INGRAM S., MUN-ZNER T.: Visualizing dimensionally-reduced data: interviews with analysts and a characterization of task sequences. In *Proceedings of the Fifth Workshop on Beyond Time and Errors:*

Novel Evaluation Methods for Visualization, BELIV 2014, Paris, France, November 10, 2014 (2014), pp. 1–8.

- [BTK11] BERTINI E., TATU A., KEIM D. A.: Quality metrics in high-dimensional data visualization: An overview and systematization. *IEEE Symposium on Information Visualization (InfoVis)* 17, 12 (2011), 2203–2212.
- [BW96] BENTLEY C., WARD M.: Animating multidimensional scaling to visualize n-dimensional data sets. In *Proceedings IEEE Symposium on Information Visualization* (1996), pp. 72 –73.
- [CH06] COVER T., HART P.: Nearest neighbor pattern classification. IEEE Trans. Inf. Theor. 13, 1 (2006), 21–27.
- [CM88] CLEVELAND W. C., MCGILL M. E.: Dynamic Graphics for Statistics. CRC Press, Inc., 1988.
- [CRMH12] CHUANG J., RAMAGE D., MANNING C. D., HEER J.: Interpretation and trust: Designing modeldriven visualizations for text analysis. In ACM Human Factors in Computing Systems (CHI) (2012), pp. 443– 452. URL: http://vis.stanford.edu/papers/ designing-model-driven-vis.
- [FA10] FRANK A., ASUNCION A.: UCI Machine Learning Repository. Irvine, CA: University of California, School of Information and Computer Sciences, 2010. URL: http:// archive.ics.uci.edu/ml/datasets/.
- [FSJ13] FERNSTAD S. J., SHAW J., JOHANSSON J.: Qualitybased guidance for exploratory dimensionality reduction. *Information Visualization 12*, 1 (2013), 44–64.
- [IMI*10] INGRAM S., MUNZNER T., IRVINE V., TORY M., BERGNER S., MÖLLER T.: Dimstiller: Workflows for dimensional analysis and reduction. In 2010 IEEE Symposium on Visual Analytics Science and Technology (VAST) (2010), pp. 3–10.
- [Ins85] INSELBERG A.: The plane with parallel coordinates. *The Visual Computer 1*, 2 (1985), 69–91.
- [IR11] ICKE I., ROSENBERG A.: Automated measures for interpretable dimensionality reduction for visual classification: A user study. In Visual Analytics Science and Technology (VAST), 2011 IEEE Conference on (2011), pp. 281–282.
- [JML12] JOSHUA M. LEWIS LAURENS VAN DER MAATEN V. D. S.: A behavioral investigation of dimensionality reduction. Proceedings of the 34th Annual Conference of the Cognitive Science Society (2012), 671–676.
- [LA11] LESPINATS S., AUPETIT M.: CheckViz: Sanity Check and Topological Clues for Linear and Non-Linear Mappings. *Computer Graphics Forum 30*, 1 (2011), 113–125.
- [MCMT14] MARTINS R. M., COIMBRA D., MINGHIM R., TELEA A.: Visual analysis of dimensionality reduction quality for parameterized projections. *Computers and Graphics* (2014).
- [PVG*11] PEDREGOSA F., VAROQUAUX G., GRAMFORT A., MICHEL V., THIRION B., GRISEL O., BLONDEL M., PRET-TENHOFER P., WEISS R., DUBOURG V., VANDERPLAS J., PASSOS A., COURNAPEAU D., BRUCHER M., PERROT M., DUCHESNAY E.: Scikit-learn: Machine Learning in Python . Journal of Machine Learning Research 12 (2011), 2825–2830.
- [SMT13] SEDLMAIR M., MUNZNER T., TORY M.: Empirical guidance on scatterplot and dimension reduction technique choices. *IEEE transactions on visualization and computer graphics 19*, 12 (2013), 2634–2643.
- [SNLH09] SIPS M., NEUBERT B., LEWIS J. P., HANRAHAN P.: Selecting good views of high-dimensional data using class consistency. In *Proceedings of the 11th Eurographics / IEEE* - VGTC conference on Visualization (2009), EuroVis'09, Eurographics Association, pp. 831–838.

- [STMT12] SEDLMAIR M., TATU A., MUNZNER T., TORY M.: A taxonomy of visual cluster separation factors. *Comput. Graph. Forum* 31, 3 (2012), 1335–1344.
- [SvLB10] SCHRECK T., VON LANDESBERGER T., BREMM S.: Techniques for precision-based visual analysis of projected data. *Information Visualization 9*, 3 (2010), 181–193.
- [SWS*99] SCHÖLKOPF B., WILLIAMSON R., SMOLA A., SHAWE-TAYLOR J., PLATT J.: Support vector method for novelty detection. *NIPS* (1999).
- [TBB*10] TATU A., BAK P., BERTINI E., KEIM D., SCHNEI-DEWIND J.: Visual quality metrics and human perception: an initial study on 2d projections of large multidimensional data. In *Proceedings of the International Conference on Advanced Visual Interfaces* (2010), AVI '10, pp. 49–56.
- [Tor52] TORGERSON W.: Multidimensional scaling: I. Theory and method. *Psychometrika* 17, 4 (1952), 401–419.
- [vdMPvdH08] VAN DER MAATEN L., POSTMA E. O., VAN DEN HERIK H. J.: Dimensionality reduction: A comparative review, 2008.
- [VPN*10] VENNA J., PELTONEN J., NYBO K., AIDOS H., KASKI S.: Infomation retrieval perspective to nonlinear dimensionality reduction. *Journal of Machine Learning Research 11*, 1 (2010), 451–490.
- [WAG05] WILKINSON L., ANAND A., GROSSMAN R.: Graphtheoretic scagnostics. In *IEEE Symposium on Information Visu*alization. INFOVIS 2005 (2005), IEEE, pp. 157–164.
- [ZL05] ZHU X., LAFFERTY J.: Harmonic mixtures: combining mixture models and graph-based methods for inductive and scalable semi-supervised learning. In *Proceedings of* the 22nd international conference on Machine learning (2005), pp. 1052–1059. URL: http://pages.cs.wisc.edu/ ~jerryzhu/publications.html.