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Interactive Tools for Explaining Multidimensional Projections for High-Dimensional Tabular Data

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A B S T R A C T

We present a set of interactive visual analysis techniques aiming at explaining data patterns in multidimensional projections. Our novel techniques include a global valuebased encoding that highlights point groups having outlier values in any dimension as well as several local tools that provide details on the statistics of all dimensions for a userselected projection area. Our techniques generically apply to any projection algorithm and scale computationally well to hundreds of thousands of points and hundreds of dimensions. We describe a user study that shows that our visual tools can be quickly learned and applied by users to obtain non-trivial insights in real-world multidimensional datasets. We also show how our techniques can help understanding a real-world dataset containing quantitative, ordinal, and categorical attributes.

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1. Introduction

High-dimensional data is present in many science and engi- neering fields and, thus, a key target for information visualization techniques. A main challenge in this respect is *scalability*, that is, how to visually depict datasets having hundreds of thousands of observations and tens to hundreds of dimensions. *Dimen- sionality reduction*, also called projection, techniques are one of the solutions of choice in this area $[1, 2]$ $[1, 2]$ $[1, 2]$. Compared to other high-dimensional visualizations such as table lenses [\[3\]](#page-14-2), paral- lel coordinate plots [\[4\]](#page-14-3), and scatterplot matrices [\[5\]](#page-14-4), projections scale well on both sample and dimension counts. As such, pro- jections have become the main technique for visualizing such data in *e.g.* biology, astronomy, chemistry, and machine learning. A raw projection is, however, just a scatterplot which does

15 not further help solving problems. As such, several methods ¹⁶ have been proposed to *explain* the visual patterns present in projections. Simple brushing and color-coding allow one to see 17 all dimensions of a single point, respectively one dimension 18 over all points. Projections can also be explained globally by 19 techniques such as biplot axes $[6, 7, 8]$ $[6, 7, 8]$ $[6, 7, 8]$ $[6, 7, 8]$ $[6, 7, 8]$ and axis legends $[9]$. 20 More recently, Da Silva *et al.* [\[10\]](#page-14-9) proposed global explanations 21 that encode how neighboring points in a projection are related $\frac{22}{2}$ to each other in terms of their dimension values. Neighborhoodbased explanations are easy to interpret (as they use the original 24 dimension names, color-coded in the projection), work with any ²⁵ projection technique, and provide information over all projected ²⁶ points. Yet, they also have important limitations [\[11\]](#page-14-10): They (1) 27 do not *scale* to more than roughly 10-15 dimensions; and (2) do ²⁸ not explain *what* the patterns in the projection mean.

Recently, Thijssen *et al.* [\[12\]](#page-14-11) extended the Da Silva *et al.* approach by observing that, for over roughly 10 dimensions, 31 providing *global* explanations for an entire projection will not ³² work – there are simply too many dimensions to color-code in $\frac{33}{10}$ the projection. They provided several mechanisms to overcome 34 the above two problems $(1,2)$ while keeping the computational 35 scalability and genericity of Da Silva *et al.* More concretely, 36

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 they proposed to (1) globally explain projection patterns by the *values* of their contained points and (2) several interactive techniques that allow scaling explanations to tens of dimensions locally. They also presented preliminary evidence from a user study showing the effectiveness of their methods.

- ⁶ In this paper, we extend the work of Thijssen *et al.* in several ⁷ directions:
- ⁸ We present mechanisms that refine the explanatory capabil-⁹ ities of the original approach;
- ¹⁰ We present a detailed analysis of a user study demonstrat-¹¹ ing the added-value of the aforementioned refinements for 12 answering complex questions on tabular data;
- ¹³ We show the added-value of our proposal by exploring a ¹⁴ complex real-world dataset containing quantitative, ordinal, ¹⁵ and categorical attributes.

 We structure our paper as follows. Section [2](#page-1-0) reviews re- lated work on projection explanations. Sections [3](#page-2-0) and [4](#page-3-0) outline our explanation extensions. Section [5](#page-6-0) details our study on the added value of our proposed mechanisms. Section [6](#page-10-0) applies our techniques for the analysis of a real-world, complex, dataset. Section [7](#page-12-0) discusses our proposal. Section [8](#page-12-1) concludes our paper.

²² 2. Related work

Let $D = {\mathbf{p}_i}$, $1 \le i \le N$, $\mathbf{p}_i = (p_i^1, \dots, p_i^n) \in \mathbb{R}^n$ be a high-
 p_i dimensional dataset with samples **p**. The values $(n^{k}1 \le i \le N)$ dimensional dataset with samples \mathbf{p}_i . The values $(p_i^k | 1 \le i \le N)$, 25 for $1 \leq k \leq n$, form the dataset's *k* dimensions. We call *D* ²⁶ *tabular* when its *n* dimensions have well-understood semantics, ²⁷ *e.g.*, they represent the measurement of a specific property that ²⁸ *D*'s analysts can reason about. Such datasets typically have a a ²⁹ few tens of dimensions [\[13\]](#page-14-12).

 A projection, or dimensionality reduction (DR) technique *P*, maps *n*-dimensional samples to *q*-dimensional ones, where ³² *q* \ll *n*. When *q* ∈ {2, 3}, the projection of a dataset *D*, denoted ³³ *D^P* = {**q**_{*i*} = *P*(**p**_{*i*})|**p**_{*i*} ∈ *D*}, can be visualized as a scatterplot. If $D^P = {\mathbf{q}_i = P(\mathbf{p}_i)|\mathbf{p}_i \in D}$, can be visualized as a scatterplot. If D^P preserves several aspects of *D* such as point relative distances or neighborhoods, then one can retrieve such *data structure* of *D* by assessing the *visual structure* of *D P* ³⁶ . Several quality metrics have been proposed to gauge projection quality, such as trust- worthiness and continuity [\[14\]](#page-14-13), false and missing neighbors [\[15\]](#page-14-14), normalized stress and Shepard correlation [\[16\]](#page-14-15), neighborhood hit [\[17\]](#page-14-16), and distance and class consistency [\[18,](#page-14-17) [19\]](#page-14-18). A recent survey [\[20\]](#page-14-19) details how to measure and interpret such metrics.

 A projection with high quelity-metric values is not *su*ffi*cient* to actually understand the projected data. Indeed, a 'raw' projection is just a scatterplot. Figure [1a](#page-1-1) shows this for a dataset containing *N* = 6500 wine samples, each having 11 measured physicochem- ical attributes and one additional dependent attribute (perceived 47 quality) [\[21\]](#page-14-20). The dataset *D* is projected to 2D using the LAMP technique [\[16\]](#page-14-15). We see some structure in this projection; what this actually means, is yet unclear.

⁵⁰ *Projection explanations* help users to assign meaning to pat-⁵¹ terns in a projection. The simplest such tool is color-coding ⁵² points by the values of a given dimension. Figure [1b](#page-1-1) color codes

Fig. 1. Wine dataset projection (a) explained by color-coding (b). See Sec. [2.](#page-1-0)

the Wine projection by its *total sulfur dioxide* dimension, showing that the bottom-right projection area has relatively higher $\frac{54}{54}$ values of this dimension. This simple explanation however cannot consider multiple dimensions.

Several other explanatory techniques exist such as biplot 57 axes [\[6,](#page-14-5) [7,](#page-14-6) [8\]](#page-14-7), axis legends [\[9,](#page-14-8) [8\]](#page-14-7), and error views [\[22,](#page-14-21) [23,](#page-14-22) [24,](#page-14-23) ⁵⁸ [15,](#page-14-14) [25,](#page-14-24) [26\]](#page-14-25). These techniques work *globally* – that is, the ex- ⁵⁹ planations they provide aim to characterize all points in a pro- 60 jection. This is challenging for local-and-nonlinear projection ϵ_{01} techniques [\[27\]](#page-14-26), such as t-SNE [\[28\]](#page-14-27) or UMAP [\[29\]](#page-14-28), which ex- $\frac{62}{2}$ hibit strong variations between how they map different data-point $\overline{63}$ nehighborhoods in D , meaning, they can hardly provide global, $\overline{64}$ accurate, explanations anchored to the visual (2D) space. A dif- ⁶⁵ ferent direction in explaining projection is given by RadViz $[30]$ 66 and related techniques [\[31\]](#page-14-30). These techniques force the projec- 67 tion to obey a given (typically circular) layout so one can relate $\overline{}$ 68 samples to dimension values. Yet, issues concerning ordering of \qquad 69 the dimensions and the global nature of the explanations persist $\frac{1}{70}$ with such methods.

Stahnke *et al.* [\[26\]](#page-14-25) combined and extended several of the π 2 above techniques. They provided an interactive tool to explore $\frac{1}{73}$ projection errors, similar to $[22, 24, 15]$ $[22, 24, 15]$ $[22, 24, 15]$ $[22, 24, 15]$ $[22, 24, 15]$, though using a different $\frac{74}{6}$ visual encoding. They also explained attribute values shared by a $\frac{75}{2}$ user-selected point set (similar to [\[10\]](#page-14-9) and follow-ups, described $\frac{76}{6}$ below). However, they require users to specifically select a point π set for explanation, whereas [\[10\]](#page-14-9) and followers do the same for $\frac{78}{8}$ all projection points. Our local explanation techniques (Sec. [4\)](#page-3-0) $\frac{79}{9}$ share many similarities with the selection-based mechanisms in $\frac{80}{20}$ Stahnke *et al.*, in particular our differential analysis tool, with $\frac{81}{100}$ the key difference that we show how the selected samples relate 82 to the *entire* dataset, not just their local distribution. Pagliosa as *et al.* [\[32\]](#page-14-31) propose a related approach. Given a point set in the 84 projection (via user interaction or data clustering), they show ⁸⁵ statistics that differentiate this set from the rest of the projection. 86 Similar to [\[10\]](#page-14-9), they consider variance of the selected attributes 87 *vs* the rest for explanation; differently, and as in Stahnke *et al.*, 88 the selection of the projection points to explain is done manually, $\frac{89}{2}$ so this approach cannot explain *all* points in a projection.

Joia *et al.* [\[33\]](#page-14-32) proposed a strategy for text document projec- 91 tions. The projection is split into clusters of points having similar $\frac{92}{2}$ data values. Next, each cluster is labeled by a tag cloud formed 93 by the most relevant keywords of the documents it contains. In 94 contrast to Stahnke *et al.*, and similar to the approach of Da 95

 Silva *et al.* (discussed below), this method explains an entire projection without requiring the user to select a subset of interest. However, setting clustering parameters to partition a projection into groups that next allow effective explanations can be tricky. Da Silva *et al.* [\[10\]](#page-14-9) explained projections by finding (and next color-coding) dimensions that contribute most to the similarity of neighbor points. In contrast to global explanations, this method adapts itself locally to show different dimensions that explain different point neighborhoods. Also, in contrast to Joia *et al.*, no explicit partitioning (clustering) of the projection is needed. Pro- posed explanations include dimension variance [\[10\]](#page-14-9), local data dimensionality [\[34\]](#page-14-33), strongest correlated dimensions [\[34,](#page-14-33) [11\]](#page-14-10), and dimension values [\[12\]](#page-14-11). All these methods address the spe- cific case of so-called *tabular* data, where the individual dimen- sions are (a) not too numerous and (b) hold specific semantics for the involved users. Yet, as Sec. [1](#page-0-0) mentions, only very limited evidence is presented on how, and whether, such explanations work for real-world datasets and users. We address this in the 19 remainder of this paper (specifically, Secs. [5](#page-6-0) and [6\)](#page-10-0).

²⁰ 3. Extending global explanations

21 Variance explanation: We first recall the variance-based expla- 22 nation of Da Silva [\[10\]](#page-14-9) which forms the basis of our extension.

Following the notations introduced in Sec. [2,](#page-1-0) let $v_i^P = {\mathbf{q} \in \mathbb{R}^n \mid \mathbf{q} \in \mathbb{R}^n \mid \mathbf$ $D^P \|\mathbf{q}_i - \mathbf{q}\| \le \rho$ be a neighborhood of radius ρ around projected
point $\mathbf{q}_i \in D^P$ Points in y^P come from the projection of a point $\mathbf{q}_i \in D^P$. Points in v_i^P come from the projection of a
peighborhood $v_i = \{ \mathbf{p} \in P | P(\mathbf{n}) \in v^P \}$ in the dataset D. They key neighborhood $v_i = {\mathbf{p} \in P | P(\mathbf{p}) \in v_i^P}$ in the dataset *D*. They key idea of Da Silva's explanation – which we take over – is that close points have similar data values, so they can be explained in terms of such data similarities. For a projected point q_i , one first computes the local variance of every dimension $1 \le d \le n$ over ^ν*ⁱ* as

$$
LV_i^d = \frac{1}{|\nu_i|} \sum_{\mathbf{p} \in \nu_i} \left(p^d - \frac{1}{|\nu_i|} \sum_{\mathbf{p} \in \nu_i} p^d \right)^2.
$$
 (1)

Next, a ranking of all *n* dimensions $\{\xi_i^d\}$, $1 \le d \le n$, is computed over y_i as over ^ν*ⁱ* as

$$
\xi_i^d = \frac{LV_i^d/GV^d}{\sum_{j=1}^n LV_i^j/GV^j},\tag{2}
$$

where GV^d is the global variance of dimension d over the entire dataset *D* computed as

$$
GV_i^d = \frac{1}{|D|} \sum_{p \in \nu_i} \left(p^d - \frac{1}{|D|} \sum_{p \in \nu_i} p^d \right)^2.
$$
 (3)

²³ Intuitively, Eqn. [2](#page-2-1) aims to capture how the variance of a dimen-²⁴ sion over a neighborhood *di*ff*ers* from the global variance of that dimension. Intuitively put, low values ξ_i^d indicate dimensions
 α *d* which vary very little over *v*. (as compared to their variance α ²⁶ *d* which vary very little over v_i (as compared to their variance over *D*), and thus are a good way to explain why points in v_i 27 ²⁸ are similar. The normalization by *GV* in Eqn. [2](#page-2-1) accounts for 29 dimensions with different variances over *D* so that low-variance ³⁰ dimensions do not get a higher ranking than high-variance ones.

The lowest-rank dimension $\lambda_i = \arg \min_{1 \le d \le n} \xi_i^d$ is picked to plain point α_i . The C most-frequent such lowest-ranks λ_i over explain point q_i . The *C* most-frequent such lowest-ranks λ_i over

the whole projection D^P are mapped to a categorical colormap with *C* colors; Less-frequent ranks are mapped to a separate 'other dimensions' color. In our work, we use the $C = 20$ colormap of Kelly [\[35\]](#page-14-34), excluding black and white. Finally, a *confidence* value C_i^d is computed for each \mathbf{q}_i and each *d*, telling how well the chosen dimension λ_i explains point \mathbf{q}_i , as

$$
C_i^d = \frac{1}{\sum_{\mathbf{q}_j \in v_i} \xi_j^d} \sum_{\mathbf{q}_j \in v_i} \begin{cases} \xi_j^d, & \text{if } d \text{ is top ranked for } \mathbf{q}_j \\ 0, & \text{otherwise} \end{cases}
$$
 (4)

that is, the rank values ξ_j^d are summed up over all points $\mathbf{p}_j \in v_j^p$
having the same top-ranked dimension as \mathbf{a}_j and the result is having the *same top-ranked dimension* as q_i , and the result is $\frac{1}{32}$ normalized by the ranks ξ_j^d summed over the entire v_i^p . The con-
 ξ_j^d fidence $C_i^{\lambda_i}$ for the lowest-rank dimension λ_i (color-mapped to 34
explain point α_i) is encoded in the point's luminance. So, bright explain point q_i) is encoded in the point's luminance. So, bright $\frac{1}{35}$ areas show cases where the color-coded dimension explains well ³⁶ many points in those areas; and conversely for dark areas. 37

Fig. 2. Variance and value explanation of a projection. (a,b) Perexplanation coloring; (c,d) Consistent coloring; (e,f) Explanations in (c,d) using the Da Silva confidence.

Value explanation: Like for variance explanation, we also compute ranks of all dimensions $\{\xi_i^d\}$, $1 \leq d \leq n$, over each neighbor-
bood *y*. The key idea behind value ranking is to find dimensions hood v_i . The key idea behind value ranking is to find dimensions
which have *outlier* values over such neighborhoods. For this we which have *outlier* values over such neighborhoods. For this, we first compute the local average

$$
LA_i^d = \frac{1}{|\nu_i|} \sum_{\mathbf{p} \in \nu_i} p^d
$$
 (5)

of dimension *d* over v_i . We next compute the value ranking of dimension *d* as dimension *d* as

$$
\xi_i^d = \frac{(LA_i^d - GA^d)/GR^d}{\sum_{j=1}^n |LA_i^j - GA^j|/GR^j},
$$
\n(6)

31

where *GA^d* is the global average of dimension *d* over *D* as

$$
GA_i^d = \frac{1}{|D|} \sum_{\mathbf{p} \in D} p^d \tag{7}
$$

and $GR^d = \max_{1 \le i \le N} p_i^d - \min_{1 \le i \le N} p_i^d$ is the range of dimension ² *d* over *D*. Note how *GR* in Eqn. [6](#page-2-2) has a similar normalization goal to *GV* in Eqn. [2.](#page-2-1) Dimensions *d* with positive ranks ξ_i^d are
a unusually high in peighborhood y_i ; dimensions with peoptive ⁴ unusually high in neighborhood $ν_i$; dimensions with negative ranks are unusually low respectively. The higher or lower the ⁵ ranks are unusually low, respectively. The higher or lower the ⁶ rank values are, the more unusual the dimension values are in a ⁷ neighborhood as compared to their averages over *D*. Depending ⁸ on the application, one can choose whether to highlight unusu-⁹ ally high (or low) dimensions, or both. For simplicity, we next ¹⁰ consider unusually high dimension values – that is, we pick the highest-rank dimension $\lambda_i = \arg \max_{1 \le j \le n} \xi_i^j$
We color man these dimensions to show the ¹² We color map these dimensions to show their identity, as for *i*¹ highest-rank dimension $\lambda_i = \arg \max_{1 \le j \le n} \xi_i^j$ to explain point \mathbf{q}_i . ¹³ variance ranking.

Robust confidence: When the ranks ξ_j^d of a top-dimension are ¹⁵ zero over an entire neighborhood, computing C_i^d will yield a ¹⁶ division by zero (see Eqn. [4\)](#page-2-3). Moreover, due to the summing of ¹⁷ ranks in Eqn. [4,](#page-2-3) confidences are skewed in different directions ¹⁸ based on the exact distribution of ranks in a neighborhood. Da ¹⁹ Silva *et al.* [\[10\]](#page-14-9) and subsequent work [\[34,](#page-14-33) [11\]](#page-14-10) fixed these issues ²⁰ by evaluating Eqn. [4](#page-2-3) on a neighborhood of larger radius $ρ_C > ρ$ than the radius *ρ* of the neighborhood *v*; used to compute ranks ²¹ than the radius *ρ* of the neighborhood $ν_i$ used to compute ranks
²² in Eqn. 2. The neighborhoods *o_C* work as a smoothing filter on ²² in Eqn. [2.](#page-2-1) The neighborhoods $ρ_C$ work as a smoothing filter on the results of Eqn. 4 – this lowers, but does not fully remove. the results of Eqn. $4 - this$ lowers, but does not fully remove, ²⁴ the chances of division-by-zero and skewness. Moreover, this 25 additional parameter ρ_c brings extra complexity for users.

We remove these problems by computing the confidence as

$$
C_i^{d, robust} = \frac{1}{|\nu_i|} \sum_{\mathbf{q}_j \in \nu_i} \begin{cases} 1, & \text{if } d \text{ is top ranked for } \mathbf{q}_j \\ 0, & \text{otherwise} \end{cases} \tag{8}
$$

 $\sum_{i=1}^{\infty}$ Simply put, $C_i^{d, robust}$ tells how often a given top-ranked dimension *d* occurs over all points in a neighborhood v_i , and has the same interpretation as Da Silva's original C^d . Our computation same interpretation as Da Silva's original C_j^d . Our computa-²⁹ tion avoids the aforementioned division-by-zero and skewness ³⁰ problems.

³¹ Figure [2a](#page-2-4) shows the variance explanation on the Wine dataset introduced in Sec. [2.](#page-1-0) Variance ranking helps explaining *why* certain projection points are close to each other – for example, all red points have similar values of the *chlorides* dimension. Dark areas, close to the borders of same-color (same-explanation) regions, indicate points where the single-dimension explanation is less confident. However, the variance explanation does not tell us *what* close points represent. The value explanation addresses this (see Fig. [2b](#page-2-4)). We see, for instance, that most red points in the variance-explanation (a), *i.e.*, wines with similar *volatile acidity* values, are now yellow, *i.e.*, are wines with unusually high *total sulfur dioxide* values.

⁴³ In the above scenario, the projection was recolored when ⁴⁴ switching explanations from variance to value. Recoloring also ⁴⁵ happens when any explanation is recomputed due to parameter ⁴⁶ changes, *e.g.* the radius value ρ used to compute the rankings in Eqs. 2 and 6. Recoloring can be confusing since the same color Eqns. [2](#page-2-1) and [6.](#page-2-2) Recoloring can be confusing since the same color

can be assigned different subsequent meanings. We solve this by 48 keeping the color allocation as consistent as possible throughout 49 such changes. At the start of the exploration, we compute an $_{50}$ initial color allocation based on the ranking mode that is in effect $\frac{1}{51}$ (variance or value). Whenever the exploration triggers an update $\frac{52}{2}$ of the dimension ranks, we compute a new color allocation, but $\frac{1}{53}$ keep dimensions that were also part of the previous explanation $\frac{54}{54}$ assigned to their earlier colors. Newly-appearing dimensions in $=$ 55 the new explanation get assigned the remaining available colors $_{56}$ based on their frequency of being top-ranked as before. $\frac{57}{20}$

Figure [2c](#page-2-4),d show this process for the variance and value ex-planations depicted in Fig. [2a](#page-2-4),b. When switching from variance $\frac{1}{59}$ to value explanation (or conversely), colors are now kept com- 60 pletely consistent. For example, the aforementioned *volatile* 61 *acidity* dimension, which was red in the variance explanation ϵ ₈₂ (a), respectively light blue in the value explanation (b), is now $\overline{}$ 63 consistently mapped to a purple color in both explanations (c,d) . ϵ

In Figures [2a](#page-2-4)-d, brightness encodes our robust confidence 65 $C_i^{d, robust}$. Figures [2e](#page-2-4),f show the same dataset with brightness 66 encoding the original Da Silva confidence C_i^d . Given that the 67 results are practically identical, and the earlier-mentioned advan- 68 tages of $C_i^{d, robust}$, we use our $C_i^{d, robust}$ further in this paper.

4. Local explanations addressing high dimension counts

Global explanations (Sec. [3\)](#page-2-0) are limited by the size C of the $\frac{71}{21}$ categorical colormap used. That is, even if we can compute $\frac{72}{2}$ explanations for many dimensions via Eqns [2](#page-2-1) and [6,](#page-2-2) we can $\frac{73}{2}$ only depict *C* of these *simultaneously*. Moreover, explaining ⁷⁴ projection patterns by a *single* dimension λ_i (whether via vari-
ance or values) only tells a small part of the full story. Indeed. ance or values) only tells a small part of the full story. Indeed, in typical projections, close points are placed so because of *mul-* 77 *tiple* dimensions. Consider *N* different clusters of points in a 78 projection. Barring any projection errors, this generally means $\frac{79}{2}$ that the dimension profiles, *i.e.*, the values that dimensions take $\frac{80}{20}$ on in those clusters, are sufficiently different from each other, 81 otherwise their points would form a single cluster. Each such 82 profile with *D* dimensions requires *D* colors to be explained. To \approx 83 fully explain the projection, all such *N* distinct dimension pro- ⁸⁴ files would need to be explained simultaneously. As *N* increases, 85 the number of dimensions that need to be explained increases. ⁸⁶

We address these limitations by several mechanisms that explain the projection *locally*. As these points, selected for local 88 explanation, are close in the projection, they are relatively similar in data values (assuming the projection is of good quality). \bullet Hence, the likelihood that they can be explained by a small $_{91}$ number of dimensions increases. Moreover, by explaining *fewer* 92 points, we can provide *more* details on these.

Figure [3](#page-4-0) shows our local explanations, which we discuss next. $_{94}$ **Lens brushing:** We select all projection points S in a given $\frac{1}{95}$ radius (adjustable via a GUI control) to the mouse pointer to be 96 the focus of the detailed (local) explanations, see next. For these $\frac{97}{20}$ selected points, we compute the variance and value rankings as ⁹⁸ for the global explanations (Eqns. [2](#page-2-1) and [6\)](#page-2-2) by substituting v_i 99 with the user selection S. Since S is fixed, in contrast to v_i which are different for every projection point *i*, we now thus compute a are different for every projection point i , we now thus compute a single variance and value ranking for all points in S – that is, we 102

Fig. 3. Local explanation of lensed points (Sec. [4\)](#page-3-0). A: Details of the explanation, including legend, for variance mode. B,C: Instances of the explanation for the variance, respectively value, modes.

explain the entire selection at once, rather than explaining every point *i* in the projection separately, as done earlier. Users can ³ interactively switch between the variance explanation (which tells *why* points in S are close in the projection) and the value ⁵ explanation (which tells *what* these points are, data-wise).

 Local analysis: We display detailed explanations of the lensed points S in a widget right to the projection. Figure [3](#page-4-0) shows this widget for a simple 3D axis-aligned cube dataset projected using PCA. The widget is structured as a table with one row per dataset dimension. For each dimension, we show its name, assigned color (by variance or value ranking, cf images (b) and (c)), and a set of statistics for that dimension, drawn right to the dimension name, described further below. In variance mode (Fig. [3B](#page-4-0)), dimensions are sorted top-to-bottom from lowest rank 15 (lowest ratio of variance in the selected points S *vs* the whole projection) to highest rank (highest ratio of variance). In contrast to the Da Silva variance explanation (Eqn. [2\)](#page-2-1), we not only show the least varying dimension (the one at the top) by color coding it in the projection, but *all* dimensions, sorted on variance over S. In value mode (Fig. [3C](#page-4-0)), we sort dimensions top-to-bottom from highest mean value in S *vs* mean value over the whole projection to lowest mean value. In contrast to the global value explanation, this shows not only the most outlier-like dimension (at top, also color-coded in the projection), but all dimensions, sorted on their outlierness. In both modes (variance and value), we thus explain the lensed points not only by a *single* (color-coded) dimension, but by *all* dimensions, sorted top-to-bottom on how important they are for the chosen explanation mode.

 Dimension statistics: The dimension sorting described above helps one find the most salient dimensions (in variance or value) ³¹ but does not explain *how much* these contribute to the lensed points S. That is, the sorting itself does not say much about

the dimension variance or values themselves. For instance, a ³³ dimension listed at the top of the value ranking may have a 34 relatively high value, or it may have a low value, as long as all ³⁵ other dimensions have even lower values. Hence, it is useful to ³⁶ show the values of the dimensions for the selected points. 37

We address this by showing both local and global statistics for 38 each dimension d in the widget. We illustrate this next for the $\frac{36}{9}$ variance mode (Fig. $3A$) – the same holds for the value mode. A 40 *range line* (same categorical color as the dimension) indicates 41 the full extent GR^d of dimension *d* over all projection points 42 from the global minimum (Fig. [3a](#page-4-0)) to the global maximum 43 (Fig. [3b](#page-4-0)). A large grey tick shows the dimension's global mean ⁴⁴ $\sum_{1 \le i \le N} p_i^d/N$ (Fig. [3c](#page-4-0)). A similar red tick shows the dimension's 45
local mean over the lensed points $\sum_{n} q_i^d / |S|$ (Fig. 3d) When local mean over the lensed points $\sum_{\mathbf{q}_i \in S} p_i^d / |S|$ (Fig. [3d](#page-4-0)) When α 46 and α and α are also the local mean is greater than the global mean we draw a green the local mean is greater than the global mean, we draw a green 47 bar between the two means to indicate a dimension having higher than usual (average) values over the lensed points. Similarly, 49 when the local mean is smaller than the global mean, we draw a 50 red bar between the two means, indicating a dimension having $\frac{51}{100}$ lower than usual values over the lensed points. The above visuals 52 show the average value of a dimension but say nothing about $\frac{1}{52}$ how its values are *spread*. This spread is important as it tells $\frac{54}{54}$ whether the dimension has a big influence on the points being 55 close together in the projection or not. Low-variance dimensions 56 for a point set result in those points having small distances $\frac{57}{20}$ in the high-dimensional space and thus, typically, also small $\frac{1}{58}$ distances in the low-dimensional embedding (projection). To $\frac{1}{59}$ convey this, we show the standard deviation of each dimension over S with white whiskers drawn left and right of the local mean $\frac{61}{100}$ (Fig. [3e](#page-4-0)). Close whiskers indicate that the lensed points vary $\overline{62}$ little over the analyzed dimension, thus the respective dimension $\overline{63}$ is important for why the points are close in the projection. This $\frac{64}{5}$ is the same information as the top-to-bottom sorting in variance $\overline{65}$ mode. However, in value mode, whiskers add the variance 66 information which is not present in that mode. Note that, while $\overline{}$ 67 our visualization is similar to a boxplot, it shows very different ϵ data: (1) our whiskers show a standard deviation, and not the $\overline{69}$ minimum or maximum values or quartiles; (2) the (green or red) π box we draw shows the difference between the global and local $\frac{71}{21}$ means of a dimension, and not quartile-related information, as $\frac{72}{2}$ in typical box plots [\[36\]](#page-14-35). $\frac{1}{3}$

Fig. 4. Differential analysis of sets of points (Sec. [4\)](#page-3-0).

 Parallel coordinates plot: All statistics discussed above are aggregates over the selected points. This can be deceiving. For example, dimensions that have the same local mean over the selected points might have quite different value distributions over the samples in S. The standard deviation whiskers show such differences but still work at an aggregated level and thus cannot convey skewed distributions or distributions with discrete value clusters. Figure [5](#page-5-0) shows an example. The selected (red) points have two dimensions with the same local mean. If we showed only this mean (a), it would be unclear if the actual distributions of the dimension values over the red points are the ¹² same.

Fig. 5. Parallel coordinate plots for the selected points (Sec. [4\)](#page-3-0).

¹³ We convey more detailed information over the selected points by drawing a PCP of all lensed points S atop of the horizontal range lines of all dimensions. To limit visual clutter, we draw the PCP half-transparent (see Fig. [5b](#page-5-0)). We now see that, while the local means of the two dimensions are the same, their value distributions are very different. Figure [5d](#page-5-0) shows the PCP lines in action for a selection of points on the already-explained cube projection (c). The *x* dimension (orange) shows near-zero values for all selected points – this is the dimension orthogonal to the cube's orange face. The *y* and *z* dimensions show, in contrast, high, respectively average, values, which are more spread out – these are the dimensions tangent to the orange face, over which the selected points have more variation and larger values.

 Differential analysis: While local explanations show detailed information over a selected projection detail, one inherently needs to explore several such details in a sequence to understand a projection. This puts a certain burden on the user's memory. We alleviate this by offering a way to *compare* two different 31 such user-selected details, as follows. The user selects a set of points S_1 , then presses a modifier key and selects a different set $33 \quad S_2$. The statistics that are normally shown in the analysis widget 34 are now replaced by statistics showing the differences between S_1 and S_2 . Figure [4](#page-4-1) shows this for the Wine dataset using the value-ranking mode. The widget shows that the two top-most dimensions (*alcohol*, pink in the projection; and *quality*, dark purple in the projection) have long green bars, while the bottom- most dimension (*density*, dark green in the projection) has a red bar. This tells that wines in S_2 have much higher alcohol and 41 quality, but lower density, than wines in S_1 .

42 **Dimension exclusion:** Local analysis allows handling higher-⁴³ dimensional data than global analysis as it shows details of all

⁴⁴ dimensions over a selected data subset. Still, datasets can con-

Fig. 6. Selective dimension disabling (Sec. [4\)](#page-3-0).

tain dimensions that do not convey much information for a given ⁴⁵ analysis. These can take up valuable colors from our limited $_{46}$ $C = 20$ categorical colormap and also clutter the explanation 47 widget. Excluding them upfront from the entire analysis is undesirable as users may wish to examine different dimension sets 49 – and keep the same projection – depending how the analysis $\frac{1}{50}$ unfolds. To address this, we allow users to click on dimensions $\frac{51}{100}$ in the widget to temporarily exclude them from the generated $\frac{1}{52}$ explanations. Doing so reassigns colors to the remaining dimensions and instantly re-creates the global and local explanations. $\frac{54}{9}$ Clicking on an excluded dimension adds it back to the generated 55 explanations. Figure [6](#page-5-1) illustrates this. In image (a), about half $\frac{56}{60}$ of the projection points are explained by unusual high values of $\frac{57}{57}$ the *diagnosis* dimension (yellow, top-most in the rank-by-value s₈ widget). To get more insight on what else makes these points different, we click on this dimension and disable it. The dimension $\overline{60}$ turns white in the widget and moves to the bottom to indicate ϵ_{61} disabling. The regenerated explanation (Fig. [6b](#page-5-1)) splits the big $_{62}$ yellow blob into differently-colored groups that provide more 63 insights of how these points differ. 64

Scalability: Our explanation system, implemented in $C++$ in 65 the ManiVault framework [\[37\]](#page-14-36), scales computationally well. It \qquad 66 computes global explanations of datasets of hundreds of thou- ⁶⁷ sands of points and hundreds of dimensions in tens of seconds, 68 and next interacts with these in real-time, on a commodity PC, $\overline{69}$ and is openly available [\[38\]](#page-14-37). Figure [7](#page-6-1) illustrates the visual scala- $\frac{70}{20}$ bility in sample (a) and dimension (b) counts. Image (a) shows $\frac{71}{10}$ a dataset consisting of 22 registered images of the same brain- ⁷² cortex tissue patch, each image mapping a gene. Pixel brightnesses encode where in the tissue the gene is expressed. We treat $\frac{74}{6}$ each pixel as a sample having 22 dimensions, one from each image. This yields $115K 22$ -dimensional samples which we project $\frac{76}{6}$ with t-SNE [\[28\]](#page-14-27) and next explain the projection. In Fig [7a](#page-6-1), the π global value explanation shows us how the projection is split $\frac{78}{8}$ into clearly separated point groups. We next lens over several $\frac{79}{2}$ points in the orange region, which corresponds to the Cux2 gene. $\frac{80}{2}$ The local explanation in the widget tells us that Cux2 is, indeed, 81 unusually high in this region (see long green bar top of widget) $\frac{1}{82}$ and that only a few other dimensions have outlier values here (all as other bars in widget are quite short). Figure [7b](#page-6-1) shows another 84 dataset [\[39\]](#page-14-38) of gene expressions in the brain cortex. This dataset 85 has 2400 samples (cells from the analyzed brain region) each 86 with 314 dimensions (gene expressions). The projection shows 87 the spatial layout of these cells. Even though the dataset has 88 hundreds of dimensions, the global value-ranking explanation is $\frac{89}{90}$ able to assign colors to unravel a salient band-like structure in \Box 90

 $\frac{1}{1}$ the projection. Using the lens, we selected points in the purple ² band (bottom in the projection). The widget tells us that these ³ have an unusually high expression of the Foxp2 gene (top-most bar in the widget), as well as showing other genes having high

⁵ expressions in this area.

Fig. 7. Scalability of explanations in number of samples (a) and dimensions (b) (see Sec. [4\)](#page-3-0).

5. Evaluation study

⁷ To evaluate the effectiveness and ease of use of our interactive system for projection explanations, we conducted a user study, which we describe next (see also Fig. [8\)](#page-7-0).

¹⁰ *5.1. Participants*

¹¹ We invited about 60 people to take part in the study (and/or 12 further spread the invitation). Of these, 23 completed the study. Participation was fully anonymous, *i.e.*, we did not collect nor trace the participants' identities. Participants self-reported (at the end of the study) experience with multidimensional data between none and several years (see also Fig. [10a](#page-7-1)).

¹⁷ *5.2. Study set-up*

 The participants were next asked to install our tool (Windows or Linux) and follow a tutorial (about 15 minutes) covering load- ing data, switching between variance and value explanations, and understanding the lens and local-explanation widget. Next, the participants were asked to analyze three multidimensional datasets and report answers via Google Forms. These datasets, all from the UCI repository [\[40\]](#page-14-39) and well-known in projection evaluation literature, had increasing dimensionalities to test our system's scalability in this respect. The *Wine* dataset was de-27 scribed already in Sec. [2.](#page-1-0) The *Cancer* dataset $(N = 569, n = 31)$

has 10 attributes describing the mean, max, and standard deviation of the size, shape, and texture values of cell nuclei in a lung $\frac{29}{29}$ tissue. The 10^{th} attribute tells whether the cells are benign or $\frac{30}{2}$ malignant. The *Spam* dataset ($N = 4601$, $n = 57$) contains fre-
quencies of selected words aiming at classifying mails as spam quencies of selected words aiming at classifying mails as spam ³² or not, and also the classification result. The datasets were projected using LAMP [\[16\]](#page-14-15) (*Wine*) and t-SNE [\[28\]](#page-14-27) (*Cancer*, *Spam*). ³⁴

5.3. Questions 35

For each dataset, participants had to answer four *control* (C) ³⁶ and three *live exploration* (LE) questions, as follows.

Control questions: The C questions involved studying screen-
sa shots of the application (produced by us) to select one of four $\frac{39}{2}$ multiple-choice answers. Answers were designed so that there 40 was a single correct one. In each screenshot, different projection points were selected by the lens; images of both global 42 and local explanations were also provided. The goal of the C_{43} questions was to see if the participants understood how to read 44 a pre-computed visualization (without interaction), explained 45 by the value mode, to come to a correct conclusion. Figure 9^{46} shows the screenshots we provided for three such questions, one 47 per studied dataset. The first question (a) shows a selection of 48 points down in the projection; we tell users that, for this dataset, ⁴⁹ we know that higher attribute values mean a higher chance of $\frac{1}{50}$ malignancy, and conversely. Users are next told that the selected $\frac{51}{51}$ points are (obviously) malignant, as they have very high levels $\frac{1}{52}$ of the *diagnosis* attribute; we see this since (1) the points are $\frac{1}{53}$ yellow and (2) the yellow-labeled attribute in the widget, called *diagnosis*, shows a green bar. This means that *diagnosis* has $_{55}$ higher values in the selection than the dataset's average. Next, users are asked which other attributes of the selected points 57 suggest that the points are *benign*. The correct answer is one 58 of the two *fractal dimension* attributes; these show red bars in 59 the widget, so they have lower values in the selection than the $\overline{60}$ dataset average. All other attributes are larger on average in the 61 selection than in the dataset (see their green bars in the widget). ϵ ₆₂

The second question (Fig. [9b](#page-7-2)) shows a selection in the Spam 63 dataset. Users are told that the selected mails are mostly spam 64 (see also the long green bar in the *spam* attribute, top in widget). 65 They are asked to tell which of the topics are likely the content 66 of these spam mail; answers include making money, advertising 67 a product, improving credit scores, or none of the above. The $\overline{68}$ correct answer is making money. Indeed, the widget shows that, 69 for the above four attributes, only *money* (second-from-top in ⁷⁰ widget) has a significant green bar, *i.e.*, this attribute has higher $\frac{1}{21}$ values in the selection than overall in the dataset. $\frac{72}{2}$

The third question (Fig. [9c](#page-7-2)) shows a selection in the Wines $\frac{73}{2}$ dataset. Users are told that the selected wines have unusually $\frac{74}{14}$ high levels of chloride (the points are red, which maps the *chlo-* ⁷⁵ *ride* attribute; and this attribute, top in the widget, has a long $\frac{1}{76}$ green bar). Next, they are asked what can be said about the π quality of the selected wines – if this is higher than average, $\frac{78}{8}$ lower than average, or nothing can be said about it. The correct answer is lower than average, since the *quality* attribute in the 80 widget (third from bottom) has a sizeable red bar.

Live exploration questions: We asked participants to analyze 82 the datasets interactively using the tool on their machines and 83

Fig. 8. Structure of the evaluation study (Sec. [5\)](#page-6-0).

Fig. 9. Three control questions for the three studied datasets (see Sec. [5.4\)](#page-7-3).

 select one or more multiple-choice answers for several LE ques- tions. We designed these questions to be harder and less clear-cut than the C ones. This, and the users' freedom to explore the visualization unconstrained, means that it is far harder to judge if an answer was 100% right or wrong. Hence, after having studied the respective datasets in depth, we ranked the LE questions' answers on an 4-point ordinal scale (very likely, likely, unlikely, very unlikely) telling how likely we ourselves would give that answer. Separately, we analyzed the coherence of the users' answers. High values tell that different people using our tool arrive at similar insights. When this occurs, we believe that the answer is likely correct since the chance that many users arrive at the same *wrong* answer is small, given their full freedom to explore the dataset.

a) Self-reported b) Control question experience answer correctness Wine Cancer Cancer Spam no experience \blacktriangleright <2 years 02. 100% 91.3% 82.6% $2-5$ years Q3. 69.6% 91.3% 95.7% \rightarrow 5 years Q4. 100% 78.3% 100%

Fig. 10. Users' experience (a) and control question answering (b).

5.4. Results 15

The 12 control (C) questions were overwhelmingly correctly $_{16}$ answered (Fig. [10b](#page-7-1)), suggesting that users were able to learn to $\frac{17}{2}$ correctly use our tool to perform low-to-medium difficulty tasks. ¹⁸

For the more complex live exploration (LE) questions, Fig. $11 \quad$ 19 shows the agreement scores. Long-and-bright bars in this figure $_{20}$ tell consensus between users and also with our own assessment. 21 Long and dark bars would indicate that many users would select $_{22}$ an answer that we consider unlikely. As Fig. [11](#page-8-0) shows, we 23 see the former bars but not the latter, which indicates a strong $_{24}$ agreement among users *and* with our assessment too. We detail ₂₅ these results next, grouping questions in terms of the type of $_{26}$ analyses they implied. For all questions, we provide our own 27 answers obtained using our tool (see Fig. [12\)](#page-9-0).

Single cluster (Q1, Wine): This relatively simple analysis asks $_{29}$ users to find very-low-density wines in the projection and find 30 which other attribute is also out-of-proportion and thus likely $\frac{31}{31}$ causes the low density. This question can be easily answered ³² using the lens and the value-ranking. Most subjects (52.2%) 33 answered *alcohol*, which is also our pick. Yet, 30.4% of the ³⁴ subjects answered here *fixed acidity*. This is potentially due to $\frac{35}{2}$ Preprint Submitted for review / Computers & Graphics (2024) 9

Fig. 11. Inter-user agreement (and our assessment of correctness likelihood) for answers of the 9 live exploration questions Q1-Q3 for all three datasets.

ambiguous phrasing of the question, which could be interpreted as having to find a dimension which deviates from the global mean in the same proportion as the density dimension. Fig-ure [12a](#page-9-0) shows our analysis for this question. We see that, indeed, ⁵ alcohol is significantly higher for the selected low-density points than all other points in the dataset.

Multiple clusters (Q1-Q2, Spam): Users were asked to find which words occurred more often in non-spam than in spam mails – thus, study at least 2 different clusters. This involved finding point clusters with spam, respectively non-spam, mails, via *e.g.* the variance global explanation, and then lensing in 12 value-ranking mode to see which of the 6 words occurred there more often than elsewhere. Participants yielded very similar answers – and also similar to our own findings. Participants were v ery close to unanimous in their answers; answers with majority votes correspond exactly with our answers. On Q1, one answer (addresses) also has several votes. This is potentially due to confusion caused by the words 'addresses' and 'address' being dimensions in the dataset, the latter of which has unusually high values in the non-spam e-mails, whereas the first does not.

21 Multiple attributes (Q3, Cancer): This question – arguably the most complex we had – involved analyzing several attributes per point cluster. This requires interactively finding projection areas having low/high values of one attribute and then analyzing the other attributes in these areas. Again, we see strong inter-user agreement and also agreement with our own findings.

 Differential analysis (Q3, Wine; Q3, Spam): Users were asked to tick up to four attributes that are most different be- tween red and white wines. To answer this, they had to find both red and white wines using the global explanation, select 31 points of these two types, and next use the differential analy-

sis to find which attributes differ between these selections. We $\frac{32}{2}$ see again a strong agreement between users and also with our-selves. Figure [12c](#page-9-0) shows our own explanation for this question. 34 We see that both *volatile acidity* and *total sulfur dioxide* have ³⁵ the largest differences followed by *fixed acidity* and *pH*. These ₃₆ results completely align with the responses of the participants. ³⁷

Dimension disabling (Q1-Q2, Cancer): Questions 1 and 2 of \quad 38 the Breast Cancer dataset asked the participants to find point 39 clusters in the projection where particular attributes had higher 40 values than all other attributes, and to note down which attributes 41 these were. Such clusters had to be found for points that were 42 completely dominated by a malignant diagnosis (high value) 43 in the diagnosis dimension, meaning all points were assigned 44 the same color (of the diagnosis dimension, see Fig. [12](#page-9-0) d1). In 45 our analysis, we found three major distinct subclusters within $\frac{46}{100}$ the point cluster with a malignant diagnosis. These were characterized by high values of the *radius*, *concave points*, and *compactness* dimensions. ⁴⁹

As Fig. [11](#page-8-0) shows, participants most commonly answered 50 *concave points* (87.0%), *radius* (78.3%), and then *compactness* ⁵¹ (43.5%) , which matches our analysis. Before going to Q2, participants were briefed on how they can disable and re-enable 53 dimensions and were told to disable the diagnosis dimension, ⁵⁴ thereby uncovering the colors of the subclusters (see Fig. $12 d2$, 55 color: value mode). We see that the *compactness* cluster is quite small and was thus harder to find for Q1. Q2 then next asked 57 participants to repeat the task of Q1 with the newly revealed 58 colour groups. In this second task, we expected participants to $\frac{1}{59}$ have an easier time finding the specific clusters as the assigned $\overline{60}$ point colors are indicating them. Given the relative small size of $\overline{61}$ the *compactness* cluster, making it hard to find in the first task ϵ ₆₂

Fig. 12. Our analysis supporting the answers of the live exploration (LE) questions. See Sec. [5.4.](#page-7-3)

without being able to see the colors, we expected it to be found

² much more often in the second task, as well as a lesser increase

³ in the other cluster attributes. Participant responses (Fig. [11\)](#page-8-0)

⁴ show the *compactness* dimension increased from selected ticked

⁵ by 43.5% of participants to 60.9% between Q2 an Q3 for the

⁶ Cancer dataset, which matches our expectations.

Fig. 13. Tool mechanisms used to answer Q2, Wine. See Sec. [5.4.](#page-7-3)

7 Dimension importance $(Q2, Wine)$: A common scenario in the analysis of real-world datasets is finding variables influencing a dependent variable. Question 2 of the Wine dataset asks the subjects to perform such an analysis by finding the region in the projection with the highest-quality wines and ticking the dimensions they believe to influence quality. Figure [11](#page-8-0) shows the recorded answers. Again, we see a good agreement of the users with our own explanation (large light bar for dimension *alcohol*). Figure [12b](#page-9-0) shows our own answer for this question. From the dimensions ranking, we see that *chlorides* has the least variance for the selected high-quality wines (since it is the top dimension in variance mode), telling that having this particular value of chlorides may be important for the high quality of the wines. Next in the ranking comes *alcohol*, and then *total sulphur dioxide* and *density*. These four dimensions are given the most votes by participants.

 Compared to the other LE questions, this question is open up to interpretation and personal judgement – finding how variables influence each other can be interpreted quite broadly. As such, we asked a follow-up question to find out how participants used our tool to reach their conclusion. Participants could report the usage of any of six predefined solutions (selected by us) or addi-tionally report a different solution via free text. Figure [13](#page-9-1) shows

the recorded answers. Interestingly, no 'other' solution was reported apart of our six options. We see the most users answered $_{31}$ the question by moving the lens over the projection and keeping 32 track of the local mean shown for the *quality* dimension. Once ³³ they found some high-quality wines, most users indicated next 34 that they ticked the dimensions that had very low variances. Our 35 own solution to answer this question was practically identical. 36

Summarizing the above, we found that participants who used 37 our tool independently and not supervised by us arrived at very $\frac{38}{100}$ similar answers of the posed questions. We deem these answers to be correct, given our own independent analysis of the 40 same datasets. While not a formal proof, we argue that this is 41 evidence that our tool can help obtaining valuable insights in 42 high-dimensional data in a predictable way.

5.5. Overall feedback ⁴⁴

Figure [14](#page-11-0) shows extra details from the participants' feedback. 45 Image (a) shows the opinions on the variance ranking. The top $\frac{46}{100}$ three bars show the answers to our questions on the usefulness 47 of this explanation (see figure for questions). Most users found 48 the variance ranking useful for finding important dimensions and 49 clusters to further explore. Yet, 13% of them found the variance $\frac{1}{50}$ ranking of no extra value. The free answers provided by the $\frac{51}{10}$ users mentioned various issues such as the ranking yielding 52 'nice' visualizations and structure to the projection; and being 53 overall interesting to explore.

Image (b) shows opinions on the value ranking. As for vari- ⁵⁵ ance ranking, most users found this mode useful to find impor- ⁵⁶ tant dimensions, clusters to explore, and extremal values. Only $\frac{57}{2}$ one user stated that this mode has no extra value; none found the 58 red-green and standard deviations bars (Sec. [4\)](#page-3-0) confusing. Free 59 answers mentioned that this mode brings additional insights; one $\overline{}$ 60 user said they would confuse this mode with variance ranking. 61

Image (c) shows opinions on the PCP plot. Most users found θ ₆₂ the plot useful to help them gauge the distribution of values $\frac{1}{63}$ in the selection and, overall, providing additional explanatory 64 value. Yet, 2 users found the plot having no extra value and $4\degree$

users that the plot makes the explanatory widget more confusing. ² Free answers mentioned that the PCP plot provides 'faint' but ³ useful cues of the data distribution; one user, though, mentioned he/she 'hates' this plot (but did not further explain why).

Images (d-g) show how users evaluated the usefulness of ⁶ all our proposed mechanisms – variance ranking, value ranking, differential analysis, and disabling dimensions, on a 7point Likert scale ranging from not very useful to very useful. Most users found overall all mechanisms useful. On the ¹⁰ above-mentioned Likert scale, we have variance mode: mean 11 score 4.83 (SD=1.63); value mode: mean score 6.52 (SD=0.77); 12 differential analysis: mean score 5.74 (SD=1.03); dimension 13 exclusion: mean score 5.74 (SD=1.42).

¹⁴ 6. Evaluation on Real-World Data

¹⁵ To bring more insights in the added-value of the proposed ¹⁶ projection exploratory techniques, we use them next to analyze ¹⁷ a more complex real-world dataset.

 Dataset: The European Values Study (EVS) dataset was created following a large-scale, cross-national and longitudinal survey, which includes a large number of questions on moral, religious, 21 social, political, occupational, and family values that have been replicated since the early eighties [\[41\]](#page-14-40). The survey goals are to measure how groups of people in Europe have similar (or different) so-called *value systems* and thereby better understand which aspects unite, respectively divide, people. This can help decisional factors at various levels to devise policy instruments to foster convergence along desirable values. The survey has 111 main questions (some with sub-questions) leading to 282 an- swers per participant. The survey which we used in our analysis was answered by 56491 citizens from 34 European countries.

31 Scalability-wise, projections can easily handle this dataset $32 \left(N = 56491 \text{ samples}, n = 282 \text{ dimensions}\right)$. Yet, *preprocessing* all 282 dimensions to make them 'compatible' for dimensionality reduction is in itself a challenge, since the dimensions are of different types (quantitative, ordinal, categorical using many different category scales); some questions allow multiple-choice answers and others not; and several questions exhibit a high frequency of missing answers. Separately, *interpreting* such projections – even with our explanatory techniques – would be very challenging since the 111 questions address widely different topics – religion, welfare, politics, role of the state, elections, education, EU enlargement, living standards, economy, and more. As mentioned earlier, our explanatory mechanisms are designed to handle tens, but not hundreds, of dimensions.

45 As such, we chose the less ambitious but more focused goal of studying only one aspect of the EVS dataset, namely ques- tions about *religious beliefs*. Table [1](#page-11-1) shows the 21 questions on this topic and their possible answers (for full details, see [\[41\]](#page-14-40)). 49 From the $N = 56491$ samples, we kept to further project the $N' = 22532$ ones which contain no missing (NA) values for any of the selected 21 dimensions. We refrained from standard techniques for imputing missing values (*e.g.* based on averages or most-frequent values) as domain specialists involved with this dataset advised us against such options which, in their experi-ence, could introduce significant biases. However, for question

v53 ('Did you ever belong to a religious denomination?'), we \sim 56 also kept samples having NA answers since this indicates people who do not describe themselves as belonging to a religious satisfying denomination. Next, we converted categorical data to numerical ss data via one-hot encoding [\[42\]](#page-14-41). Finally, we normalized all quan- 60 titative variables to the range [0, 1] by standardization (subtract 61) the mean, divide by standard deviation): and weighed the sets of the mean, divide by standard deviation); and weighed the sets of $\overline{6}$ one-hot-encodings that map one categorical variable by $1/\sqrt{2}$, as
so they have a proportional contribution to the total similarity so they have a proportional contribution to the total similarity $\overline{}$ 64 function as the quantitative variables. $\frac{65}{65}$

Results: Figure [15](#page-13-0) shows the t-SNE projection of the EVS $\frac{66}{66}$ dataset colored by variance. Image (a) shows the overview. The 67 projection consists of well-separated point clusters which suggest a clear grouping of the respondents based on their religionrelated answers. We see some coarse-level structure: Several 70 central groups (light blue) indicate people with no religious de- ⁷¹ nomination. We also see several light-purple groups at different $\frac{72}{2}$ places on the outskirts the projection. These are people who $\frac{73}{2}$ answered similarly to $v9$ (are you in a church/religious organization?) Since there are several such groups, the answers to $v9$ 75 are different (some are and some are not in such organizations) π and/or other factors exist that differentiate them.

To get more insight in the projection, we select a few groups $\frac{78}{8}$ for further analysis. Image (b, red points) shows such a group to $\frac{79}{20}$ the bottom. The widget tells us that these are, compared to the 80 dataset's average, people more present in church organizations, 81 who more often believe in God, heaven, hell, and the afterlife, say and go to church more often. Interestingly, they have a wide $\frac{1}{83}$ spectrum of beliefs concerning the form God takes $(v62)$. We \approx can cautiously describe them as 'institutionally religious' people. ⁸⁵ Image (c) selects a cluster top-left in the projection. Its widget, $\frac{1}{100}$ and the earlier-observed purple color in image (a) , tell us that $\frac{1}{87}$ these are also people in religious organizations. Yet, the top 88 green bars in the widget show that, compared to the dataset 89 average, they don't believe in afterlife, God, heaven, and hell, 90 but strongly believe children should have religious faith and 91 overall believe God is important. We can describe such people ₉₂ as formally non-religious but supporting the ethical importance $\frac{1}{93}$ of religion. Finally, image (d) explores a cluster just right to ⁹⁴ the one in image (c). Comparing its widget with that of (c) we $\frac{1}{95}$ see that the second bar from the top (believe in reincarnation, 96 $v61$) changes a lot: These are people who do not believe in $\frac{97}{20}$ reincarnation, while those selected in (c) did, with all their other attributes being roughly similar.

Figure [16](#page-13-1) shows the projection explained by outlier values. 100 Image (a) uses the same colormap as Fig. [15a](#page-13-0). We get more 101 insights into the projection structure: The right yellow groups 102 share outlier answers to $v6$ (whether religion is important). The 103 middle purple groups, overlapping many of the light-blue groups 104 in Fig. [15a](#page-13-0), have outlier answers to $v9$ (whether in a religious 105 organization). Bottom-left, brown groups have outlier answers 106 to prayer frequency outside religious services $(v64)$. Finally, the 107 top-left green groups have outlier answers to whether religious 108 faith is desirable for children $(v93)$.

Let us re-examine the same selected groups as in Fig. [15b](#page-13-0)-d 110 via outlier values. Figure [16b](#page-13-1) shows that people in the bottom 111 group pray (outside of religious services) significantly less, and ¹¹²

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 a) Variance ranking assessment b) Value ranking assessment

a) Variance ranking assessment b) Value ranking assessment Helps find important dimensi (52.296) Helps find important dimension $-15(65.2%$ Helps find clusters to explore Helps find clusters to explore $-22(957%$ No extra value 211296 Helps find very high values $-20(87%$ $(1.4.3\%)$ Helps find very low values 12 (52.2%) (4.3%) Red/green bars ar confusing Stddev bars are confusing $-1(4.3\%)$ $-1.64.3%$ free answers $-1(4.3%)$ No extra value $-0(0%$ $(4.3%)$ $-1(4.3%$ free answers ${^{+}}{\rm{14.3\%}}$ $\left\{\begin{array}{ccc} -1.4.3\% & -1.4.3\% \\ -1.4.2\% & -1.4.3\% \end{array}\right\}$ **c) PCP plot assessment d) Usefulness of variance ranking** Helps gauge distr. of values AA AAR ONLY Provides extra expl. value 14 (80.004) No extra value Makes widget more confusing $-4.117.496$ $-1.64.3%$ $1(4.3%)$ free answers $-1.64.396$ $(4.3%)$ $\frac{1}{2}$ $\frac{1}{2}$ $\frac{3}{4}$ $\frac{5}{5}$ $\frac{8}{10}$ very useful **e) Usefulness of value ranking f) Usefulness of differential analysis g) Usefulness of disabling dimensions** 0.00%

not very useful 2 3 4 5 6 very useful not very useful 2 3 4 5 6 very useful not very useful <u>2 3 4 5 6 very useful</u> Fig. 14. Details of our user evaluation concerning questions about our techniques' overall perceived added-value. See Sec. [5.5.](#page-9-2)

Table 1. Questions and representations of answers of 21 religion-related opinions from the EVS dataset. See Sec. [6.](#page-10-0)

¹ believe in spirits significantly less, than the dataset average. This matches well our earlier description of 'institutionally religious' people. Figure [16c](#page-13-1) confirms our earlier findings from Fig. [15c](#page-13-0). The bars in the widgets of these two figures are the same. What differs is the sorting order: In variance mode (Fig. [15c](#page-13-0)), bars are sorted from low to high variance, allowing us to find the least varying, thus most homogeneous, dimensions over a selection; in value mode (Fig. [16c](#page-13-1)), bars are sorted from high to low out- lierness, allowing us to find dimensions having unusually high (or low) values in a selection. The added-value of the two modes becomes clear when we examine Fig. [16d](#page-13-1), where we selected the same group as in Fig. [15d](#page-13-0): As explained earlier, the differ- ence of this group and the one left of it is immediate when we compare the widgets in Figs. $16c,d$ – the variance sort shows the belief in reincarnation (orange dimension, second-top) changes a lot between the two widgets, telling what makes the groups

different. In value mode, this dimension is the one-but-last in 17 Fig. [16c](#page-13-1) but pops second-to-top in Fig. [16d](#page-13-1). Hence, variance 18 sort helps more to explain the differences of these two groups. 19

The scenarios involving images (c,d) in Figs. [15](#page-13-0) and [16](#page-13-1) aim to \approx 20 find what differentiates two point groups. We can complete this $_{21}$ task also by the differential analysis tool (Sec. [4\)](#page-3-0). Consider the \qquad 22 three small groups selected in red at the center of Fig. [16e](#page-13-1). The $_{23}$ widget tells us that these are people not in church organizations ₂₄ (long green bar at top) but who, interestingly, do believe in hell $_{25}$ and reincarnation much more than the dataset average (long 26 red bars at the bottom). What differentiates these three groups 27 *from each other*? To answer this, we select first the top two 28 groups (A and B) and use the differential tool (Fig. [16f](#page-13-1)). The ²⁹ widget now shows a single long red bar at the bottom, telling $\frac{30}{2}$ that group B has people who believe far more in heaven than $\frac{31}{21}$ the ones in group A. All other bars are relatively short, so this $\frac{32}{2}$

belief in heaven is *the* main differentiator of these two groups. Next, we select groups B and C and use again the differential ³ tool (Fig. [16g](#page-13-1)). The widget shows a long green and a long red bar, telling that people in cluster C believe far less in the afterlife, but believe far more often in heaven, than people in group B. Finding such differentiators between point groups would have been significantly harder without the differential tool that shows what makes them, pair-wise, different.

Assessment: We ran our findings with an expert who has a strong background in both infovis and the social sciences domain from which the dataset emerges, and was not involved in the development or testing of our tool. Our questions were (a) whether our explanatory techniques have the potential to show currently-unknown insights on these data; and (b) whether our visualization (projection plus interactive explanations) do make sense and are superior to the common tools known by experts ¹⁷ in their domain. The answers to both questions were clearly positive: (a) The findings we highlighted earlier in this section were unknown to researchers in the field *and* were also deemed interesting and worthy of further analysis; (b) there were no similar tools known in the expert's domain which could allow researchers to explore the EVS data in the way we did – the closest tool they would know of is a (t-SNE) projection annotated by the values of a *single* dimension selected by users (which, as shown in Sec. [2](#page-1-0) and Fig. [1,](#page-1-1) clearly does not scale to more than a few dimensions). While this evidence is not enough to draw strong conclusions, we believe it offers sufficient ground to assert that our proposal is of potential added-value to scientists aiming to explore high-dimensional datasets via explained projections.

30 7. Discussion

³¹ We next discuss several key aspects of our proposal.

32 Genericity: Our proposed explanatory methods are generic – ³³ they work for any projection technique *P* and high-dimensional dataset *D*, including data having quantitative, ordinal, and cate-³⁵ gorical attributes (see Sec. [6\)](#page-10-0), as long as one has a (good quality) ³⁶ projection of the data to explore.

37 Scalability: Our explanatory methods only require the compu-³⁸ tation of variance-and-value metrics over relatively small point ³⁹ neighborhoods in the projection (Eqns. [1](#page-2-5) and [5\)](#page-2-6). These are 40 *O(κNn)* for *N* dataset points having *n* dimensions and *κ* points α ₁₁ in the local neighborhood of radius *o* in a projection (see Sec. 3) ⁴¹ in the local neighborhood of radius ρ in a projection (see Sec. [3\)](#page-2-0)
⁴² – and trivially to parallelize in a SIMD manner. – and trivially to parallelize in a SIMD manner.

⁴³ Ease of use: Using our explanatory techniques is easy as out-⁴⁴ lined by the presented study in Sec. [5.](#page-6-0) All our users, having quite ⁴⁵ diverse backgrounds, were able to understand our techniques 46 and apply them to find correct results on three relatively complex ⁴⁷ datasets and questions in several tens of minutes.

 Limitations: Our proposal has several limitations. First, as stated in Secs. [1](#page-0-0) and [2,](#page-1-0) we only address *tabular* data, which contains a limited number of dimensions *n* (roughly, tens) that 51 all have clear semantics for the user. If dimensions do not have a clear meaning for users, using them to explain a projection does not make much sense. A related limitation is that we cannot handle data with *missing values*. This can significantly decrease

the applicability of our method to the full extent of informa-tion present in real-world datasets (see Sec. [6\)](#page-10-0). While we can $_{56}$ argue that handling missing values is out of the scope of our 57 explanatory techniques for projections, it is definitely interesting to think how one could meaningfully 'insert' such values 59 into a projection or, alternatively, complete the statistics shown $\overline{60}$ by our explanatory widgets by all valid attributes present in a 61 dataset. Secondly, our local explanations (Sec. [4\)](#page-3-0) are also limited in showing statistics over the brushed selection – averages, $\overline{}$ 63 ranges, standard deviations, and parallel coordinate plots. These 64 simple to interpret signals are by no means exhaustive. Find- 65 ing more involved (summarized) descriptions of what makes a $_{66}$ neighborhood 'particular' is an open research topic. Finally, our 67 differential tool allows comparing two neighborhoods at a time $\overline{68}$ (Sec. [4\)](#page-3-0). It is definitely interesting to extend this to compare θ multiple such neighborhoods.

8. Conclusion $\frac{71}{21}$

We have presented a set of interactive visual techniques for $\frac{72}{2}$ the exploration and explanation of multidimensional projections. $\frac{73}{2}$ Our techniques include local and global value-based explana- ⁷⁴ tions, detailed statistics on all dimensions, comparing projection $\frac{75}{6}$ regions, and dimension filtering. Our techniques can generically $\frac{76}{6}$ handle any projection algorithm and scale computationally and τ visually to datasets of over 100K samples and over 300 dimensions. A user study showed that our techniques can be quickly $\frac{79}{29}$ learned, are found useful, and can be applied to answer nontrivial questions involving real-world multidimensional datasets, 81 and lead to similar findings from different users for the same 82 datasets and questions. We also showed that our techniques can as be applied to complex, real-world, datasets containing attributes of mixed type – ordinal, categorical, and quantitative – to unravel 85 hitherto unknown insights from the respective datasets.

Several directions can be explored next. Global explanations, although useful, are still limited as they inherently show a *single* set dimension. Further studying the original idea proposed – but not elaborated – by Da Silva [\[10\]](#page-14-9) to use dimension-sets, possibly $\frac{1}{90}$ complemented by dimension-value-ranges, has strong potential 91 to improve the added value of such explanations. Separately, we 92 could incorporate knowledge on the specific projection method 93 used to make the explanatory metrics more insightful than using 94 generic variance and outlier-value computations. Also, both 95 our global and local analyses can be enhanced to support more 96 targeted queries, $e.g.$ 'show me other projection regions similar \Box to this selected one'. Finally, deploying our tool in a long-term 98 analysis scenario involving a real use-case and domain experts $\frac{99}{99}$ would bring additional evidence for its practical value.

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Fig. 15. Variance explanation of the EVS dataset. (a) Overview showing the main variables that explain the projection clusters. (b-d) Details for three selected clusters. See Sec. [6.](#page-10-0)

Fig. 16. Value explanation of the EVS dataset. (a) Overview showing the main variables that explain the projection clusters. (b-d) Details for three selected clusters. (e-g) Differential analysis of three small clusters in the center. Insets right of each projection show our local explanation widgets. See Sec. [6.](#page-10-0)

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