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Visual Exploration of 3D Shape Databases via Feature Selection

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Abstract: We present a visual analytics approach for constructing effective visual representations of 3D shape databases as projections of multidimensional feature vectors extracted from their shapes. We present several methods to construct effective projections in which different-class shapes are well separated from each other. First, we propose a greedy heuristic for searching for near-optimal projections in the space of feature combinations. Next, we show how human insight can improve the quality of the constructed projections by iteratively identifying and selecting a small subset features that are responsible for characterizing different classes. Our methods allow users to construct high-quality projections with low effort, to explain these projections in terms of the contribution of different features, and to identify both useful features and features that work adversely for the separation task. We demonstrate our approach on a real-world 3D shape database.

1 INTRODUCTION


Recent developments in 3D content creation and 3D content acquisition technologies, including modeling and authoring tools and 3D scanning techniques, have led to a rapid increase in the number and complexity of available 3D models. Such models are typically stored in so-called *shape databases* (ShapeNet, 2019; ITI DB, 2019). Such databases offer next various mechanisms enabling users to browse or search them to locate models of interest for a specific application at hand.


As shape databases increase, so does the difficulty that users have in locating models of interest therein (Tangelder and Veltkamp, 2008). Typical mechanisms offered to support this task include searching by *keywords*, browsing the database along one or a few predefined hierarchies, or content-based shape retrieval (CBSR). While efficient for certain scenarios, all these mechanisms have limitations: Keyword search assumes a good-quality labeling of shapes with relevant keywords, and also that the user is familiar with relevant search terms. Hierarchy


browsing is most effective when the organization of shapes follows the way the user wants to explore them. Finally, CBSR works well when the user aims to search for shapes similar to an existing query shape.


Besides the above targeted use-cases, more generic ones involve users who simply want to *explore* the *entire* database to see what it contains. This is relevant in cases where users want to first get a good overview of what a database contains before deciding to invest more effort into exploring or using it; and also in cases where users do not have specific searches in mind. Existing mechanisms offered for the above scenarios are linear in nature, showing either a small part of the database at a single time and/or asking the user to perform lengthy navigations to create a mental map of the database itself, much like when navigating a web domain.

We address this task by a different, visual, approach. We construct a compact and scalable *overview* of an entire shape database, with shapes organized by similarity. We offer *details-on-demand* mechanisms to enable users to control the separation quality of the similar-shape groups in the visual overview; understand what makes a set of shapes similar (or two or more sets of shapes different); and find features that have high, respectively little, value for the shape classification task. Our approach is simple to use; requires no prior knowledge of the orga-

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nization of a shape database; nor a prior organization or labeling of the database; handles any type of 3D shape represented by a polygon mesh; and scales visually and computationally to real-world large shape databases. Additionally, our proposal is useful for both end users (who aim to explore a shape database) and technical users (who aim to engineer features to query or classify shapes in such databases).

This paper is structured as follows. Section 2 outlines related work in exploring 3D shape databases. Section 3 details our pipeline that consists of shape normalization, feature extraction, and dimensionality reduction. Section 4 presents our automatic and user-driven methods for constructing high-quality projections for exploring shape databases, and demonstrates these on a real-world shape database. Section 6 concludes the paper.

2 RELATED WORK

Searching and exploring 3D shape databases can be structured along three modalities, as follows.

Keyword search uses words to search for shapes whose annotation data contains those words. It is the simplest to support, and therefore oldest and most widespread form of search for 3D content, present in many shape databases, such as TurboSquid (TurboSquid, Inc., 2019) and Aim@Shape (Aim@Shape, 2019), to mention just a few. Such databases allow providers to upload models with associated keywords for subsequent search. However, keyword lists are only weakly structured, possibly containing redundant or vague keywords, potentially added this way to increase exposure rate. Besides general-purpose databases of this type, more specialized ones exist, such as containing 3D shapes related to space exploration (NASA, 2019). Overall, keyword search is popular and widely supported, but works best for targeted searches performed by users aware of a database’s organization, require a good annotation with specific keywords, and is less effective for overall exploration.

Hierarchical exploration systems organize shapes along different criteria, following an existing taxonomy of the targeted 3D shape universe at hand. Such systems support exploration (apart from keyword search) by allowing users to browse the hierarchy, with shapes or shape categories depicted by thumbnails, much like when exploring a file system. Examples of such systems are the Princeton Shape Benchmark (Shilane et al., 2004), Aim@Shape (Aim@Shape, 2019), or the ITI 3D search engine (ITI DB, 2019) that allows browsing

multiple hierarchically-organized shape databases. Hierarchy browsing supports browsing better than keyword-based search. Yet, it typically only allows examining a single path (shape subset) at a time, and cannot provide a rich global overview of an entire database. Moreover, its effectiveness relies on the provided hierarchy, which may or may not match the way users see the grouping of shapes.

Content based shape retrieval (CBSR) allows users to search for shapes similar to a given query shape, and therefore depend far less on an upfront organization of the database in terms of suitable keywords or hierarchies and/or on the user’s familiarity with these. Good surveys of CBSR methods are provided by (Bustos et al., 2005; Tangelder and Velkamp, 2008). These methods essentially extract a high-dimensional descriptor from the query and database shapes, and then search and retrieve the most similar shapes to the query based on a suitable distance metric in descriptor space. Many types of descriptors and distance metrics have been proposed, as follows. Global descriptors, such as shape elongation, eccentricity, and compactness, are simple, yet crude ways to discriminate between highly different shapes. Local descriptors, such as saliency, shape thickness, and shape contexts capture more fine-grained shape details (Shtrom et al., 2013; Rusu et al., 2009; Shapira et al., 2008; Tasse et al., 2015). Topological descriptors, such as based on curve skeletons (Jalba et al., 2012) or surface skeletons (Feng et al., 2016) capture the part-whole shape structure. Finally, view-based descriptors capture the appearance of the shape from multiple viewpoints (Cyr and Kimia, 2001; Shen et al., 2003). Kalogerakis *et al.* (Kalogerakis et al., 2010) provide a tool to compute several types of shape features. Apart from such hand-engineered descriptors, deep learning has proved effective in automatically extracting low-dimensional representations of shape with high accuracy for query tasks (Su et al., 2015). CBSR frees the user from the burden of specifying keywords or choosing explicit navigation paths in a hierarchy to examine a shape database. Additionally, CBSR assists in finding the most similar shapes to a given prototype (query). However, CBSR does not readily support the task of general-purpose exploration of a shape database, *e.g.*, seeing how *all* the shapes within it are organized in terms of similarity.

Summarizing the above, keyword search, hierarchical exploration, and CBSR offer largely complementary mechanisms for exploring a shape database, and can be readily combined in a 3D database exploration system. However, as outlined, none of these methods offer a compact, complete, and detailed overview of an entire database. Moreover, such mech-

anisms do not explain *why* a set of shapes are deemed similar. In earlier work, Rauber *et al.* (Rauber et al., 2015) have used interactive feature selection to improve image classification, which is related, but not the same, to our goal of *exploring* data collections. Such functionalities are essential in contexts where users do not know precisely what they are looking for, and would like to understand the information contained in a database before proceeding to more specific queries.

3 PROPOSED METHOD

To support the overall exploration of 3D shape databases, we propose to *augment* existing mechanisms (keyword search, hierarchies, and CBSR) by a visual navigation approach. Our approach allows users to see a complete overview of an entire database and the way shapes are organized within in terms of similarity. Next, it allows selecting specific shapes or shape properties and finding similar shapes (from the perspective of one or several such properties), and also finding out how properties discriminate between different shapes. We now detail our approach.

3.1 Overview

We start by introducing some notations. A mesh $m = (V = \{\mathbf{x}_i\}, F = \{f_j\})$ is a collection of vertices $\mathbf{x}_i \subset \mathbb{R}^3$ and faces f_j , assumed to be triangles for simplicity. A shape database is a set of shapes $M = \{m_k\}$. No restrictions are placed here, *i.e.*, shapes can be of different kinds, sampling resolutions, and require no extra organization or annotations, *e.g.*, classes or hierarchies.

Our key idea is to present a visual *overview* of M in which every shape m_k is represented by a thumbnail rendering thereof, and visual distances between two shapes m_i and m_j reflect their similarity. The visual overview is interactively linked with detail views in which users can explore specific shape details. The combination of overview and details, following Shneiderman’s visual exploration mantra (Shneiderman, 1996), enables both free and targeted exploration of the shape database along the use-cases outlined in Sec. 2.

We create our overview-and-detail visual exploration as follows. First, we preprocess all meshes in M so as to normalize them in terms of sampling resolution and size. Secondly, we extract local features from all meshes $m \in M$ (Sec. 3.3). These features capture the respective shapes at a fine level of detail. Next, we aggregate local features into fixed-

length feature vectors (Sec. 3.4). Finally, we use a dimensionality-reduction algorithm to project the shapes, represented by their feature vectors, onto 2D screen space (Sec. 3.5). We describe all these steps next.

3.2 Preprocessing

Since we do not pose any constraint on the shapes in M , these can come with virtually any sampling resolution, orientation, and at any scale. Such variations are known to pose problems when computing virtually any type of shape descriptor (Bustos et al., 2005). Hence, as a first step, we normalize all shapes $m \in M$ by first remeshing them, with a target edge-length of 1% of m ’s bounding-box diagonal. Next, we translate and scale the remeshed shapes to fit the $[-1, 1]^3$ cube.

3.3 Local Feature Extraction

To characterize shapes, we extract several so-called *local features* from each. Such features describe the shape at or in the neighborhood of every vertex $\mathbf{x}_i \in m$ and are therefore good at capturing local characteristics. We compute seven local feature types, as follows.

Gaussian Curvature (Gc): Gaussian curvature describes the overall flatness of a shape close to a given point. For every vertex $\mathbf{x} \in m$ we compute its Gaussian curvature as

$$Gc(\mathbf{x}) = 2\pi - \sum_{f \in F(\mathbf{x})} \theta_{\mathbf{x},f}, \quad (1)$$

where $F(\mathbf{x})$ is the set of faces in F incident with \mathbf{x} and $\theta_{\mathbf{x},f}$ is the angle in face f at vertex \mathbf{x} .

Average Geodesic Distance (Agd): We estimate the geodesic distance $d(\mathbf{x}, \mathbf{y})$ between a pair of vertices \mathbf{x} and \mathbf{y} of m as the geometric length of the shortest path in the edge connectivity graph of m between \mathbf{x} and \mathbf{y} . This distance can be easily and efficiently estimated using Dijkstra’s shortest-path algorithm with A* heuristics and edge weights equal to edge lengths. More accurate estimations of the geodesic distance between two points on a polygonal mesh exist, including computing the distance field (or transform) $DT(\mathbf{x})$ of \mathbf{x} over F and tracing a streamline in $-\nabla DT(\mathbf{x})$ from \mathbf{x} until it reaches \mathbf{y} (Peyre and Cohen, 2005); GPU minimization of cut-length using pivoting slice planes passing through \mathbf{x} and \mathbf{y} (Jalba et al., 2013); or hybrid search techniques (Verma and Snoeyink, 2009). While more accurate than the Dijkstra approach we use, these methods are *considerably* more complex to implement, slower to run, and require careful tuning and/or specialized platforms (GPU support). For a detailed comparison of

geodesic estimation methods on polygonal meshes, we refer to (Jalba et al., 2013). More importantly, we do not use the *individual* geodesic lengths, but aggregate them into per-shape feature vectors (Sec. 3.4). As such, high geodesic estimation precision is less important.

Given the above, we estimate the average geodesic distance of a vertex \mathbf{x} as

$$Agd(\mathbf{x}) = \frac{\sum_{\mathbf{y} \in V} d(\mathbf{x}, \mathbf{y})}{|V|}. \quad (2)$$

Normal Diameter (Nd): We first estimate the surface normal at a vertex \mathbf{x} as

$$\mathbf{n}(\mathbf{x}) = \sum_{f \in F(\mathbf{x})} \mathbf{n}(f) \theta_{\mathbf{x}, f}, \quad (3)$$

where $\mathbf{n}(f)$ is the outward normal of face f . Given the above, let \mathbf{r} be a ray starting at \mathbf{x} and advancing in the direction $-\mathbf{n}(\mathbf{x})$. The normal diameter $Nd(\mathbf{x})$ is then the distance along \mathbf{r} from \mathbf{x} to the closest face $f \in F \setminus F(\mathbf{x})$.

Normal Angle (Na) and Point Angle (Pa): These features describe how vertices $\mathbf{x} \in V$ are spread around the shape itself. In detail, let \mathbf{e}_1 be the dominant eigenvector of the shape covariance matrix given by all vertices V . As known, \mathbf{e}_1 gives the direction in which the shape spreads the most. Next, for every vertex $\mathbf{x} \in V$, we define the normal angle $Na(\mathbf{x})$ as the angle (dot product) between \mathbf{e}_1 and the surface normal $\mathbf{n}(\mathbf{x})$; and the Point Angle $Pa(\mathbf{x})$ as the angle (dot product) between \mathbf{e}_1 and the vector $\mathbf{c} - \mathbf{x}$, where \mathbf{c} is the barycenter of m .

Shape Context (Sc): The shape context descriptor is a 2D histogram that characterizes how vertices of a shape are ‘seen’ in terms of distance and orientation from a given vertex of that shape (Belongie et al., 2001). For a vertex $\mathbf{x} \in V$, the shape context describes the number of vertices in V that are within a given distance range and direction range to \mathbf{x} . To compute Sc , we first build a local coordinate system at every vertex \mathbf{x} , using the eigenvectors of the shape covariance matrix in the neighborhood of \mathbf{x} . This ensures that this coordinate system is aligned with the shape locally — one of its axes will be the normal $\mathbf{n}(\mathbf{x})$, whereas the two other ones are tangent to the surface of m at \mathbf{x} . Next, we discretize the orientations around \mathbf{x} into the eight octants of the local coordinate system, and distances using a set of bins (distance ranges) (t_i, t_{i+1}) defined by a distance-set $T = \{0, t_1, t_2, \dots, t_n, 1\}, n \in \mathbb{N}_+$. In practice, we use $T = [0, 0.1, 0.3, 1]$. Hence, for each vertex \mathbf{x} , we get a shape context vector with $8 \times 3 = 24$ elements.

Point Feature Histogram (PFH): PFH (Rusu et al., 2009) is a complex descriptor that captures the local geometry in the vicinity of a vertex. Given a pair of

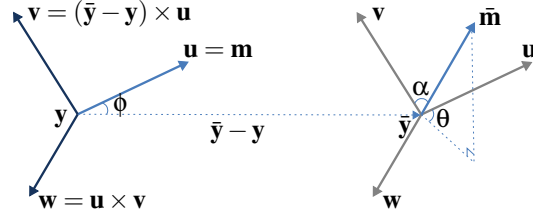


Figure 1: PFH descriptor computation (Shtrom et al., 2013).

vertices \mathbf{y} and $\bar{\mathbf{y}}$, one first defines a local coordinate frame $(\mathbf{u}, \mathbf{v}, \mathbf{w})$ as

$$\begin{aligned} \mathbf{u} &= \mathbf{m}, \\ \mathbf{v} &= (\bar{\mathbf{y}} - \mathbf{y}) \times \mathbf{u}, \\ \mathbf{w} &= \mathbf{u} \times \mathbf{v}, \end{aligned} \quad (4)$$

where \mathbf{m} is the vertex normal at \mathbf{y} (Fig. 1). Next, the variation of the shape geometry between points \mathbf{y} and $\bar{\mathbf{y}}$ is captured by three polar coordinates

$$\begin{aligned} \alpha &= \mathbf{v} \cdot \bar{\mathbf{m}}, \\ \phi &= \mathbf{u} \cdot \frac{\bar{\mathbf{y}} - \mathbf{y}}{\|\bar{\mathbf{y}} - \mathbf{y}\|}, \\ \theta &= \arctan2(\mathbf{w} \cdot \bar{\mathbf{m}}, \mathbf{u} \cdot \bar{\mathbf{m}}), \end{aligned} \quad (5)$$

where $\bar{\mathbf{m}}$ is the vertex normal at $\bar{\mathbf{y}}$. Next, three histograms are built to capture the distributions of α, ϕ, θ for a given vertex \mathbf{x} by considering all pairs $(\mathbf{y}, \bar{\mathbf{y}}) \in N_{\mathbf{x}, k} \times N_{\mathbf{x}, k}$ in the k -nearest neighbors $N_{\mathbf{x}, k}$ of \mathbf{x} . In practice, we set $k = 30$ and use 5 bins for each histogram. This delivers a PFH feature vector of $5^3 = 125$ entries.

Fast Point Feature Histogram (FPFH): While PFH models a neighborhood $N_{\mathbf{x}, k}$ by all its point-pairs, the Simplified Point Feature Histogram (SPFH) models $N_{\mathbf{x}, k}$ by the characteristics of the pairs $(\mathbf{x}, \mathbf{y} \in N_{\mathbf{x}, k})$. We proceed analogously to binning the α, ϕ, θ distributions in three histograms of 11 bins each, obtaining a feature vector of $3 \times 11 = 33$ elements. With this vector, we finally compute the FPFH value of a vertex \mathbf{x} following (Rusu et al., 2009) as the distance-weighted average of the SPFH values over the neighborhood $N_{\mathbf{x}, k}$ as

$$FPFH(\mathbf{x}) = SPFH(\mathbf{x}) + \frac{1}{k} \sum_{\mathbf{y} \in N_{\mathbf{x}, k}} \frac{SPFH(\mathbf{y})}{\|\mathbf{x} - \mathbf{y}\|}. \quad (6)$$

3.4 Feature Vector Computation

The features described in Sec. 3.3 are *local*, i.e., they take different values for every mesh vertex $\mathbf{x} \in V$. To be able to compare meshes to each other, we need to reduce these to same-length *global* descriptors. For this, we use a simple histogram-based solution that aggregates the values of every local descriptor, at all

vertices of a mesh, into a fixed-length (10 bin) histogram. Note that some descriptors are by definition high-dimensional — for instance, the shape context Sc has 24 dimensions. Hence, for a d -dimensional descriptor, we compute a histogram having $10d$ bins. Table 1 shows the local features, their dimensionality, and the number of bins used to quantize each. Summarizing, we reduce every shape m to a 1870-dimensional feature vector \mathcal{F} .

3.5 Dimensionality Reduction

So far, we have reduced a shape database M to a set of $|M|$ 1870-dimensional feature vectors. We next create a visual representation of the shape database by projecting all these vectors onto 2D using the well-known t-SNE dimensionality reduction method (van der Maaten and Hinton, 2008). Simply put, t-SNE constructs a 2D scatterplot $P(M) = \{P(m_k)\}$, where every shape $m_k \in M$ is represented by a point $P(m) \in \mathbb{R}^2$, so that the distances between scatterplot points reflect (encode) the similarities of their feature vectors.

An important concern when proposing such a representation is to gauge its *quality*. To do this, we use the classes (labels) of the shapes. For a database where each shape m has a categorical label $c(m) \in C$, where C is a set of categories (e.g., keywords describing the different shapes in a database), we define the neighborhood hit $NH(m)$ as the proportion of the k -nearest neighbors of $P(m)$ that have the same label $c(m)$ as m itself (Paulovich et al., 2008). In practice, we set $k = 10$, following related applications that gauge projection quality (Paulovich et al., 2008). With this, we can next define the neighborhood hit of an entire class $c \in C$ as

$$NH_c(c) = \frac{\sum_{m \in M: c(m)=c} NH(m)}{|\{m \in M : c(m) = c\}|}. \quad (7)$$

Finally, at the highest aggregation level, we define the neighborhood hit for an entire scatterplot $P(M)$ for a

Table 1: Local features, their dimensionalities and binning.

Name	Dimensionality	Bins
Gaussian curvature (Gc)	1	10
Average geodesic distance (Agd)	1	10
Normal diameter (Nd)	1	10
Normal angle (Na)	1	10
Point angle (Pa)	1	10
Shape context (Sc)	24	240
Point Feature Histogram (PFH)	125	1250
Fast Point Feature Histogram (FPFH)	33	330
Total		1870

shape database M as

$$NH_s(M) = \frac{\sum_{m \in M} NH(m)}{|M|}. \quad (8)$$

The above two NH metrics describe how a mesh (point in the 2D projection scatterplot) is separated from points of different kinds: NH_c shows whether a group of points representing same-class meshes is well separated in a scatterplot (something we desire since we want next to use the scatterplot to answer the question “How many shape classes are in a database, and how similar are they to each other?”). NH_s shows how well a whole scatterplot can represent an entire shape database. Both NH metrics range between 0 and 1, with higher values indicating better separation, which is preferred.

4 APPLICATIONS

We next demonstrate our visual exploration approach on a subset of the Princeton Shape Benchmark (Shilane et al., 2004) having 280 meshes from 14 classes, with 20 meshes from each class. As outlined earlier, these meshes are not labeled, hierarchically organized, or otherwise preprocessed.

4.1 Optimal Scatterplot Creation

The projection scatterplot (Sec. 3.5) is the central view that shows an entire shape database. Hence, creating a good scatterplot is important for all exploration tasks addressed next. In this section, we explore the following questions:

- Q1: How can we create a good projection scatterplot?
- Q2: Which features are best for grouping similar shapes (and, conversely, separating different shapes) in the scatterplot?
- Q3: Which is the minimal set of features required to generate a good-quality scatterplot?

Concerning Q1, we could directly create and examine a t-SNE projection of the whole shape database as encoded by the 1870-dimensional feature vectors we extracted (Sec. 3.4). However, using t-SNE is not always easy, especially for high-dimensional data: This method maps similarities (of feature vectors) *non-linearly* to 2D distances; also, tuning t-SNE’s parameters to yield a good embedding of high-dimensional feature vectors is notoriously hard (Wattenberg, 2016). Hence, we first explore the simpler solution of projecting only *subsets* of all extracted features. As we have 8 feature types (Tab. 1), a natural idea is to try all combinations of

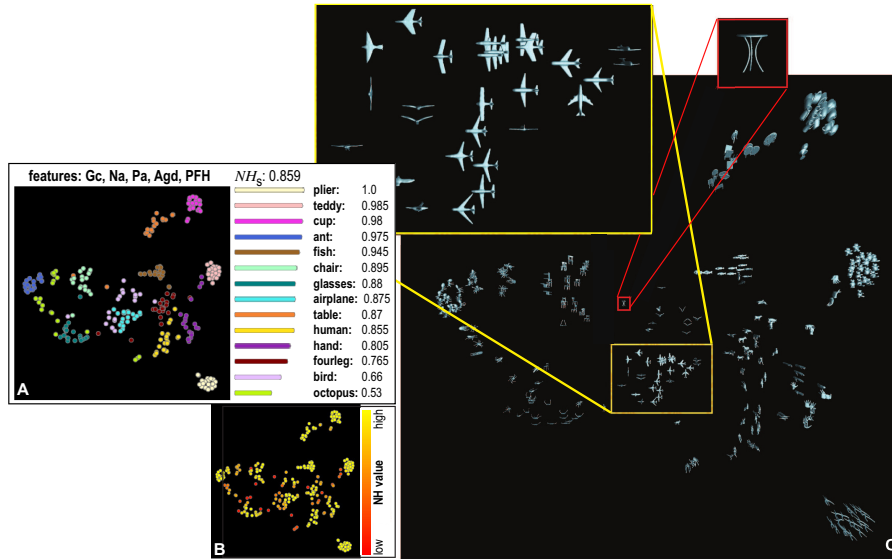


Figure 2: Three views of the optimal projection scatterplot for the Princeton Shape Database, depicting classes and their NH_c values and the overall plot quality NH_s (A), per-shape NH values (B), and actual shape thumbnails (C).

groups of feature types. This yields $2^8 - 1 = 255$ possible projection scatterplots. Following the scagnostics idea (Tukey and Tukey, 1988; Wilkinson et al., 2006), we compute all these scatterplots (using t-SNE) and select the one having the highest quality, measured by its NH_s value.

Figure 2 shows three views of the optimal projection scatterplot, as follows. Image A shows the scatterplot with points (shapes $m \in M$) colored by their class value $c(m)$. The text atop this image indicates the feature subset leading to this optimal scatterplot (highest $NH_s = 0.859$ value), namely (Gc, Na, Pa, Agd, PFH). The bar chart in image A shows the NH_c values for all classes, with high values (well separated classes) at the top. From this, we can see that *pliers* are perfectly separated from all other classes ($NH_{pliers} = 1$), while *octopus* is least well separated ($NH_{octopus} = 0.53$). Image B shows the optimal scatterplot colored by NH values for all shapes, ranging between red (low NH) to yellow (high NH). Red points in this image show shapes which are not projected well — that is, placed close to shapes having different classes. Finally, image C shows the optimal scatterplot with shapes depicted by thumbnails. From this image, we find that shapes of the classes *pliers*, *teddies*, *cups*, *ants*, and *fishes* are well projected. However, *birds* are mixed with *airplanes*; and *fourlegs* are mixed with *humans* and *hands*. The *octopus* class is visually split in the projection into several parts. While this optimal scatterplot is not perfect, it is *still* formally the best one we can create given the combinations of our 8 available features. Indeed, while class separation is not perfect, closely-projected shapes are still quite similar. For instance, *ants* are surrounded by

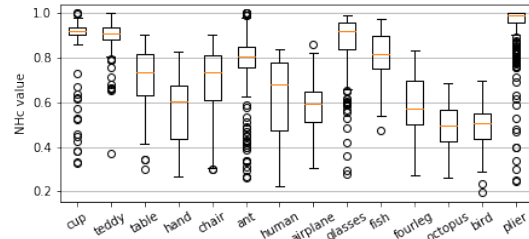


Figure 3: NH_c statistics for the 14 classes in the shape database for all considered 255 projection scatterplots.

octopuses, which is arguably logical, since both shape types have many thin and spread legs. Similarly, *airplanes* and *birds* are close to each other; indeed, both have wings and are relatively flat.

Figure 3 shows boxplot statistics of the NH_c values for the 14 shape classes in our database for the 255 created projection scatterplots. Ideally, we would like to see that every class has a very high NH_c value. However, we see that *birds* and *octopuses* have quite low NH_c values, confirming the insights obtained earlier by visually examining the projection (Fig. 2).

Finally, Fig. 4 shows a complete view of how features affect the quality of the produced projections. The bar chart shows the NH_s values of all possible 255 projections created by combining our 8 features types, sorted in increasing values from left to right. The matrix plot below the bar chart shows which features (color coded according to the legend at the right) are used by which projection. Projections using more than one feature have blue bars; projections that use exactly one feature have their bars colored by the respective feature. This plot gives us several insights:

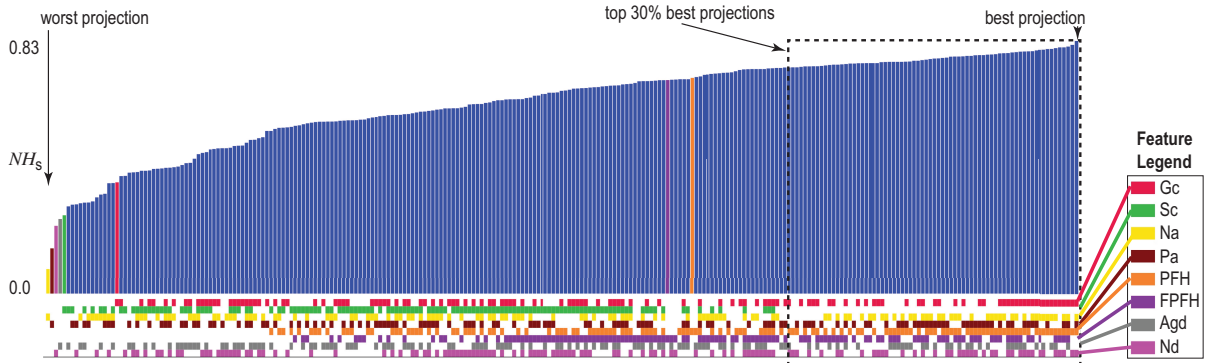


Figure 4: A bar chart showing the NH_s scores of 255 projections, sorted on increasing value (best projections to the right, worst ones to the left). The color blocks under a bar show which features are used for that projection (the feature color legend on the right). Bars which are not blue only use one feature, whose identity colors the bar. Scanning the color matrix below the bars row-wise tells us which projections use which features. We see that PFH (orange) and FPFH (purple) are good features since their blocks are close to the right. Conversely, Sc (green) is not a very useful feature since its blocks are spread to the left.

(1) The quality difference between the best and worst projections is significant (NH_s 0.831 vs 0.38), with better projections using more features than poor ones; (2) some features are really instrumental in achieving high quality, *e.g.* PFH (orange) and FPFH (purple), which appear consistently in the right of the matrix plot in Fig. 4, whereas other features are actually adversely affecting quality, *e.g.* Sc (green) which appears in the left of the matrix plot. This indicates either that Sc is not a useful feature for discriminating classes in this database or that it is poorly evaluated, *e.g.*, by an insufficiently dense sampling. (3) Overall, the right of the matrix is more full than its left part, which means that using more features produces better segregating projections, although the relation is not monotonic. (4) The highest-quality projections (roughly, rightmost third of the bar chart) consistently use the same mix of features (Gc, Na, Pa, PFH, FPFH, Agd, Nd). (5) The patterns in the matrix plot of different features look different, which means there are no redundant features in the considered set.

4.2 Fast computation of near-optimal projection scatterplot

Computing all possible scatterplots given a feature vector \mathcal{F} to find the optimal one is expensive, especially when the set \mathcal{F} is large. We next propose a greedy algorithm to accelerate this task (Alg. 1). The parameter s gives the maximum size of the feature-set to search for. For every search iteration, $\binom{s}{|\mathcal{F}|}$ feature combinations are examined, and the best one, in terms of the realized NH_s value, is retained. Better solutions are obtained for larger s values, at the expense of longer search times. When $s = |\mathcal{F}|$, Alg. 1 compares all possible $2^{|\mathcal{F}|}$ feature combinations. From

our tests, a quite good solution in terms of NH_s value can be found by setting $s = 1$. For this setting, the time complexity of our algorithm is $O(|\mathcal{F}|^2)$.

Table 2 shows the results of our greedy algorithm, executed 5 times, to account for the stochastic nature of the t-SNE projection. For every round, we indicate the time taken by exhaustive search vs our greedy search, and also the number of t-SNE projections being evaluated. We see that our algorithm yields practically the same NH_s quality as the exhaustive search, but is roughly 5 times faster.

Algorithm 1 Computing near-optimal feature sets.

Input: Set of features \mathcal{F} ; maximal size s , $1 \leq s \leq |\mathcal{F}|$, of feature-set to search for,
Output: Near-optimal feature set C ,
1: $C := \emptyset, C_{new} := \emptyset$;
2: **repeat**
3: $C := C_{new}$
4: **for each** $\mathcal{F}_{sub} \subseteq \mathcal{F}, |\mathcal{F}_{sub}| \leq s$ **do**
5: $C_{temp} := (C \cup \mathcal{F}_{sub}) - (C \cap \mathcal{F}_{sub})$
6: **if** $NH_s(C_{temp}) > NH_s(C_{new})$ **then**
7: $C_{new} := C_{temp}$;
8: **end if**
9: **end for**
10: **until** $(C_{new} = C)$;
11: **return** C ;

4.3 User-Driven Projection Engineering

Section 4.2 showed how we can automatically select features from the eight existing feature classes (Tab. 1) to create a projection scatterplot which best separates shapes from different classes. However, using this automatic approach has some disadvantages: (1) It is *expensive*, even when using the proposed greedy algorithm for feature selection. (2) It is too

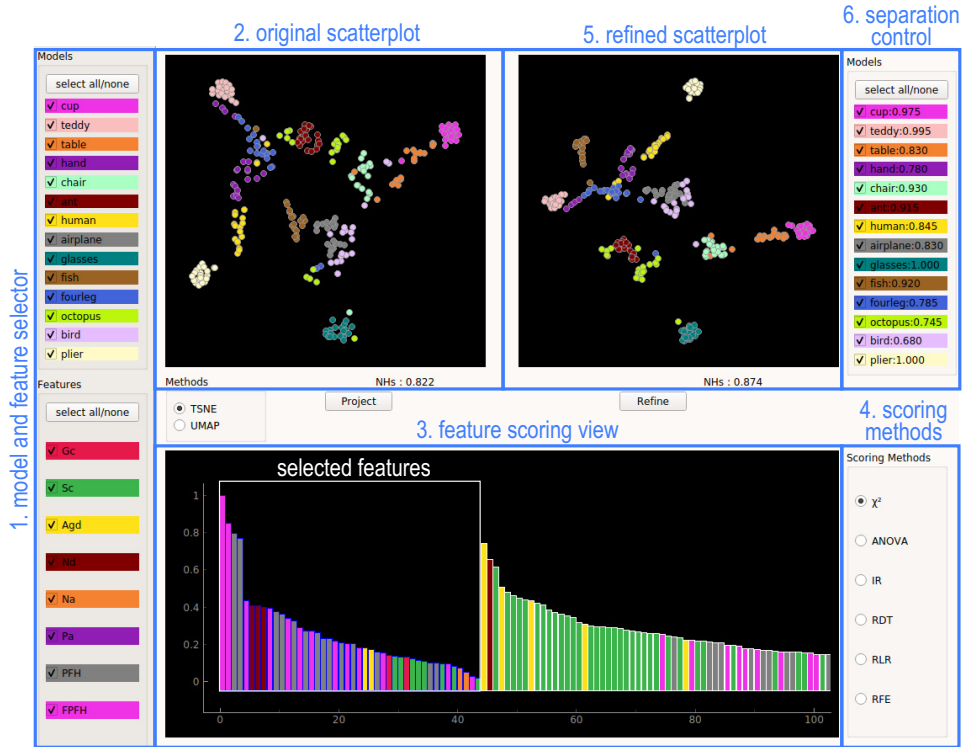


Figure 5: A user-driven projection engineering tool and its six views (Sec. 4.3).

coarse-grained: All features of the same *type*, e.g., the 24 shape-context Sc features are either selected all, or ignored, when constructing the projection. (3) It is too *simplistic*: There are cases when, for instance, we want to optimize for separation of certain classes more, based on problem-specific constraints. Hence, *user input* in deciding which feature combination leads to the optimal projection is crucial.

We next address question Q2, rephrased as: How can we pick ‘good’ feature-bins (from the total set of 1870 bins) that separate classes in the way we desire *in a specific context*? For this, we propose an interactive tool based on feature scoring (Fig. 5) which contains several views (1–6) that allow the user to explore the effect of features on separating classes of shapes

Table 2: Performance of the greedy algorithm.

Round	Search method	NH_s	Time (secs)	t-SNE runs
1	Exhaustive	0.831	459.74	255
	Greedy	0.831	103.49	56
2	Exhaustive	0.830	452.12	255
	Greedy	0.830	84.98	48
3	Exhaustive	0.829	453.70	255
	Greedy	0.820	70.24	40
4	Exhaustive	0.832	445.47	255
	Greedy	0.832	111.71	64
5	Exhaustive	0.824	447.66	255
	Greedy	0.824	97.39	55

in the database, and also select subsets of features that lead to a desired, better, class separation. We explain these views via an overview-and-details-on-demand workflow, as follows:

Model and feature selector (1): The user starts by selecting the shape classes and feature types of interest in this view. This allows them to specify if they are interested in separating specific classes (which are then to be selected) or, alternatively, interested in separating equally well all classes from each other (in which case, all classes should be selected). For instance, from our earlier experiments discussed in Sec. 4.1, we saw that birds are hard to separate from airplanes. The user can then select only these two classes in view (1) to explore how to increase their separation. Separately, one can select the feature types (of the 8 computed ones) to use for creating the scatterplot. This is useful to examine, or debug, the effect of a specific feature type. Classes are categorically color-coded, and the same colors are used in the scatterplots (2, 5). Similarly, feature types are categorically color-coded with the same colors used in the feature scoring view (3).

Original scatterplot (2): This view shows a scatterplot using all shape classes *vs* all feature types chosen in the selector (1). It acts as a starting point for the exploration, which can next be refined to e.g. pro-

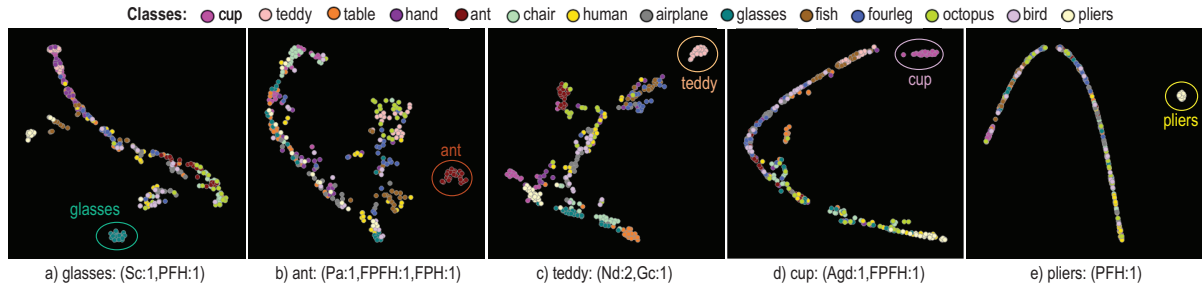


Figure 6: Finding minimal number of feature-bins able to separate five shape classes from the rest of the database. Notation $name:i$ indicates that i bins of feature $name$ are used.

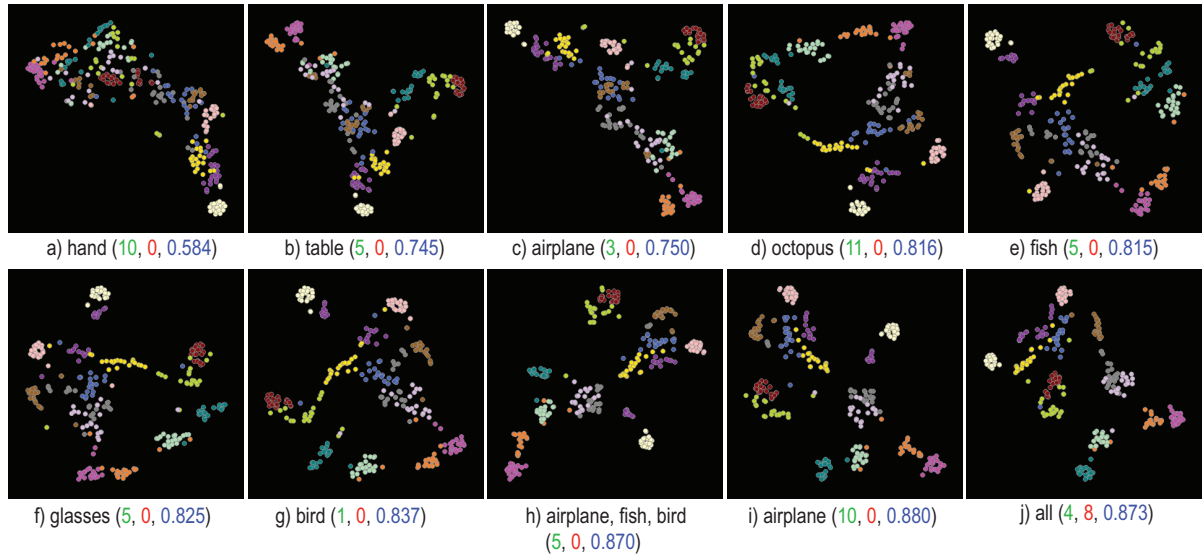


Figure 7: Incremental creation of high-quality projection scatterplot that separates all classes well. In each step, a few feature-bins (having high scores, count indicated in green) are selected to separate one or several classes from the rest, and a few feature-bins (having low scores, count indicated in red) are removed from the selection. NH_s at each step are rendered blue.

duce better separation of desired classes or instances (shapes) using the feature scoring views (3, 4) discussed next. Scatterplots can be computed either with the t-SNE or UMAP (McInnes et al., 2018) projection methods. t-SNE spreads similar points better over the available 2D space, but takes longer to compute. UMAP creates denser clusters separated by more whitespace, but is faster to execute. For a trade-off of these two techniques, we refer to a recent survey (Espadoto et al., 2019).

Feature scoring views (3, 4): Each bar in the bar chart (3) shows the *discriminative score* of every element f_i of the 1870-dimensional feature vector, *i.e.*, how much f_i contributes to separating class c_i from a few or from all other classes $c_j \neq c_i$ selected for exploration in view (1), depending on the separation control (6, discussed later). Colors identify to which feature types the elements f_i belong. For instance, the several purple bars in Fig. 5(3) correspond to the 330 bins that the FPFH feature (colored purple in Fig. 5(1)) has. Scores are computed with six scor-

ing methods (Rauber et al., 2015): chi-squared, one-way ANOVA, Randomized Decision Trees (RDT), Randomized Linear Regression (RLR), iterative relief (IR), and Recursive Feature Elimination (RFE), which can be chosen by the user in panel (4). The bar chart supports two tasks: First, it shows how the many bins that each feature is represented by contributes to the separation power of that feature. Secondly, it allows fine-grained examination of the effect of each such bin on the class separation: Users can freely *select* specific bins (from the 1870 available ones) to create a new projection. The selected bins are displayed with a blue border and listed, in decreasing score order, before the unselected ones, in the bar chart. The new projection created by the user-selected bins is shown in view (5).

Refined scatterplot (5): This scatterplot shows instances from the classes selected in view (1), projected according to the specific feature-bins selected in the bar chart (3). This is thus a *refined view* of the original projection (1). By comparing the re-

finer scatterplot with the original one, one can thus see how fine-grained selection of every single of the 1870 feature-vector components can improve the projection or parts thereof. In other words, obtaining an optimal projection is achieved in two steps: First, one can select entire features (in view 1). This corresponds to considering or ignoring entire *features* that capture different aspects of shape. Upon obtaining a suitable projection, one can refine it by selecting or deselecting individual bins for the selected features. This corresponds to considering or ignoring *ranges* of the values of the features under exploration.

Separation control (6): As mentioned, feature scoring measures how well selected features separate a class c_i from one or several classes $c_j \neq c_i$. The view (6) allows controlling this. The view shows all shape classes c_i in the database. If all classes are selected in view (6), scoring will measure how well a class c_i is separated from *each* of the other classes $c_j \neq c_i$. If only one class c_i is selected in (6), then scoring will measure the separation of c_i from $\cup_{j \neq i} c_j$. This way, one can flexibly measure the separation of arbitrary *groups* of classes rather than only the separation of individual classes themselves.

4.4 Use-cases

We demonstrate the added value of our user-driven projection engineering by answering several practical questions, as follows.

A. What is the minimal number of feature values, and which are these, that are sufficient to separate a given class of shapes from all others (Q3, Sec. 4.1)?

Figure 6 illustrates this use-case for the classes glasses (a), ant (b), teddy (c), cup (d), and pliers (e). For each class, we select the respective class in the model selector (Fig. 5(1)) and use next the feature scoring view (Fig. 5(3)) and separation control (Fig. 5(6)) to find the feature values (bins of the 1870-dimensional feature vector) that best separate this class from the remaining ones. We assess separation both visually, using the refined projection (Fig. 5(5)) and its corresponding NH_s score. We find, this way, that these classes can be separated very well from the rest of the database by a *maximally three*, and sometimes just one, feature bin(s) of the 1870 computed ones, as indicated in Fig. 6. This is, we believe, a quite powerful (and novel) result as it indicates that very little computational effort is needed for classifying shapes in the Princeton Shape Database (and, by extension, in other similar databases). In turn, this can considerably increase the scalability of applications such as shape retrieval and classification.

B. How can we explain the discriminatory power of

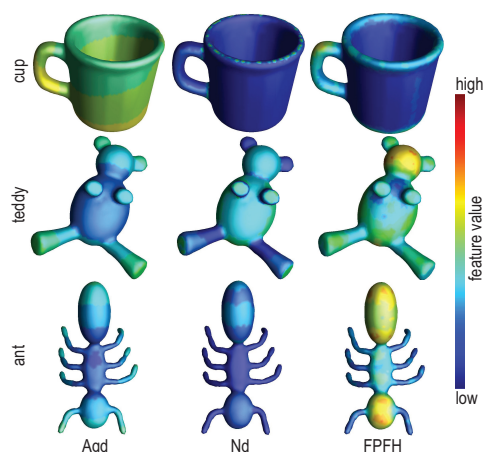


Figure 8: Feature-bins (Agd 6th bin, Nd 1st bin, and FPFH 6th bin) mapped on three shapes. This shows how these specific feature bins can effectively separate these shapes.

the features found in use-case A?

The computed feature scoring and the clear separation shown in the refined projection scatterplots (Fig. 6) are, in principle, enough to let us choose the minimal set of feature-bins needed to separate a class from all others. However, it is useful to double-check and explain this discriminatory power, to ensure that the features found this way indeed reflect meaningful different properties of the respective shape classes. For this, we choose shapes from the analyzed classes in use-case A and color them by the values of the features found in the same step to be strongly characteristic of specific classes. Figure 8 shows this for three such shapes and feature-bins, respectively. As visible, the three feature-bins take indeed different values for the three shapes. Atop of this insight (which we already knew from the analysis shown in Fig. 6), we also see now that the Nd feature has indeed low values on thin shape parts and large values on thick ones, respectively. Similarly, we see that the Agd is large for shape protrusions (*e.g.* ant and teddy legs) but is small for central shape parts (*e.g.* teddy rump). The FPFH feature is harder to interpret visually; still, we can see how it gets high values on roughly round shape parts (teddy head and ant's first and last segments) and low values elsewhere.

C. How can we create a good scatterplot which separates well all classes?

Figure 7 shows an example workflow for this task. We start here with a scatterplot that uses all 1870 features. Next, we search, using the feature scoring view (Fig. 5(3)), for the feature-bins that are most discriminatory, *i.e.*, have highest scores, for each of the classes in our database, starting with the hand class (we could start from any other class). As we progress investigating subsequent classes, we add feature-bins which are

discriminatory for these newly visited classes. At the end, when we have considered all classes, we also remove features, from the already added ones, which have low scores (that is, bring the least discrimination value or even work adversely for this task). The entire process can be done in one to two minutes. The different images in Fig. 7 show us how the quality (NH_s value) of the scatterplot almost monotonically improves as we add more feature-bins by considering new classes. Note that, in this process, we may visit a certain class several times (e.g. airplane), as features that score high for it may appear several times during the exploration as we add other classes. The final result (Fig. 7j) contains all 14 classes, has a value $NH_s = 0.873$, and is obtained with a total set of 51 feature-bins. Note that this final NH_s value is *higher* than the one we found by the exhaustive search ($NH_s = 0.831$, Tab. 1). Indeed, our manual search is more fine-grained, as it allows us to consider individual *feature-bins* (of the 1870 in total), whereas the automatic search only considered entire *features* (of the 8 in total). Also, note that obtaining this result by exhaustive search would be prohibitively expensive, as this would involve searching all 2^{1870} combinations.

5 DISCUSSION

We discuss next several aspects of our method, as follows:

Dimensionality reduction: Currently, we directly reduce dimensionality of our 1870-dimensional feature vector to 2D using either t-SNE or UMAP. However, this may be too hard a task for these projection methods to perform, while in the same time preserving neighborhoods. Another approach is to use more dedicated methods, such as autoencoders, to reduce dimensionality to a lower value, and then project this low-dimensional dataset to 2D using t-SNE or UMAP. However, it has to be checked whether this approach can yield final 2D scatterplots that better preserve the structure of the shape database. Concerning the choice of projection techniques, we used t-SNE and UMAP as these techniques are known for their ability to separate well, in the visual space, clusters of similar observations, as opposed to other projection techniques (Espadoto et al., 2019).

Scalability: Our method depends on two key parameters in this respect, namely the number of *shapes* in the database to be explored, and the number of *features* which are extracted from each shape. From a computational viewpoint, feature extraction can be done offline, as shapes are changed and/or new shapes are added to the database. Since, typically, shape

databases do not change with a high frequency, such an offline extraction can be done without impeding the performance of the end user. Moreover, features can be extracted in parallel, both among themselves and over different shapes. We compute the t-SNE projection using the *scikit-learn* implementation, which projects several hundreds of instances in a few seconds; the UMAP implementation, provided by the authors (McInnes et al., 2018), works in real time for this dataset size. If needed, other, faster projections can be used (Pezzotti et al., 2017). From a visualization viewpoint, the scatterplot, barchart, and matrix plot metaphors we use scale well to hundreds of thousands of points (shapes) and tens of features.

Evaluation: One important aspect concerning our proposal is evaluating its effectiveness for different types of tasks and users. In detail, we identify *end users*, for whom tasks involve getting an overview of a shape database, finding similar groups of shapes, finding which features make two shape groups similar (or different), and finding outlier shapes; and *technical users*, for whom tasks involve selecting a small set of features able to create effective visualizations for the first user group. We consider such evaluations to be part of future work.

6 CONCLUSION

We have presented an interactive visual analytics system for exploring 3D shape databases for CBSR applications. After reducing shapes to high-dimensional feature vectors following standard feature extraction, we visualize the similarity structure of a database by using dimensionality reduction. To this end, we offer several mechanisms for creating projections in which different shape classes are separated well from each other. First, we use a scagnostics approach to generate near-optimal projections based on maximizing the quality of resulting projections, using a greedy heuristic to optimize the search for suitable feature-sets. Next, we propose a visual analytics approach to enable users to select a small feature subset for separating specific classes, generate high-separation projections for all classes, and gauge the separation power (thus, added-value) of all available features. We show that this visual analytics approach allows generating projections with better separation quality than automatic approaches, and also helps finding both discriminating features (to be used in a CBSR system) and confusing features (of little value for such systems). Our approach can be applied to any 3D shape database and feature-set, allowing CBSR engineers to streamline the process of design-

ing and selecting effective features for shape classification and retrieval. We demonstrate our work on a real-world 3D shape database.

Several extensions of this work are possible, as follows. First and foremost, performing a user study to gauge how well our approach can support exploration tasks of typical end users, is an important addition. Secondly, since our approach is generic, it could be used to optimize feature selection in other applications beyond CBSR, *e.g.*, in image classification.

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