

Local Data Models for Probabilistic Transfer Function Design

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Abstract

A central component of expressive volume rendering is the identification of tissue or material types and their respective boundaries. To perform appropriate data classification, transfer functions can be defined in high-dimensional histograms, removing restrictions of purely 1D scalar value classification. The presented work aims at alleviating the problems of interactive multi-dimensional transfer function design by coupling high-dimensional, probabilistic, data-centric segmentation with interaction in the natural 3D space of the volume. We fit variable Gaussian Mixture Models to user specified subsets of the data set, yielding a probabilistic data model of the identified material type and its sources. The resulting classification allows for efficient transfer function design and multi-material volume rendering as demonstrated in several benchmark data sets.

Categories and Subject Descriptors (according to ACM CCS): I.3.0 [Computer Graphics]: General—

1. Introduction

Volume rendering is used in fields such as medicine [PB07] and engineering and relies on the definition of transfer functions, which map properties of scalar data to visual properties such as color. If the visualization goal is the display of distinct materials, transfer functions are effectively a classification technique that serves as input to a rendering stage.

The design of transfer functions is complex even for low-dimensional domains and is therefore, since it typically cannot be performed fully automatically, often offloaded to the user. In an interactive setting, these transfer functions can be designed by operating in spaces such as a histogram [KD98], a correlation space [BM10], or a topological abstraction [BPS97]. Here, raising the dimensionality of the histogram domain allows for better data classification but at the same time fundamentally increases the complexity of interactive transfer function design. In more than two dimensions visual representations of the domain and interaction techniques become complex and increasingly non-intuitive.

This paper proposes a technique to decorrelate classification power and interactive design complexity by utilizing unsupervised learning and probabilistic classification. We hide conceptual complexity of high-dimensional transfer function design from the user by modeling the classification procedure as one-class classification based on user-specified samples of the volume data. As the user selects such a set of voxel samples, an unsupervised learning approach mod-

els the selected samples as set of random variables originating from multiple probabilistic sources by performing adaptive Gaussian Mixture Model (GMM) fitting. As a result, a complex classifying data model is learned while the user selects part of the data directly in 3D and performs iterative classification of the data set. This query-driven approach reduces the complexity of interaction operations by hiding computational complexity from the user while at the same time achieving multi-dimensional data classification. In summary, our work makes the following contributions:

- Non-global, high-dimensional, and probabilistic transfer function design in 3D
- Iterative query-driven, local data model specification
- Local data model estimation with mixed GMMs

2. Motivation and Related Work

Scalar data may be classified into materials based on property selection in 1D (e.g., scalar histograms [Lev88]), or higher-dimensional spaces (as defined by derived properties such as gradient, curvature [SWB*00], locality [LLY06, CQC*08], correlation [BM10], and other measures [KKH02, KVUS*05, HPB*10]). However, due to noise, measuring inaccuracies, and other effects, meaningful features in the volume data do not necessarily correspond to generic features in histogram space. In multi-dimensional histograms, specific data models may be used to identify histogram features with data features (cf. arcs in gradient-

intensity histograms [KD98]). However, generic data models for automatic classification are rare.

Fortunately, humans are capable to interpret desired results in volume classifications easily [MAB*97], implying user-guided data model generation outside of histogram space as a solution to this problem. For basic transfer functions the user is able to identify approximate features directly in the volume rendering - whereas automatic classification [MWCE09, WZL*12, IVJ12] is clearly superior when operating in the high-dimensional histograms. For this reason, we propose the unification of interactive image centric classification and automatic data centric classification as an approach for efficient multi-dimensional volume classification. A number of works have aimed at providing means for effective (semi) interactive transfer function design. Direct modification of global transfer function properties in 3D was proposed by Guo et al. [GMY11]. In other work, unsupervised learning of two-class classification by *Neural Networks* or *Support Vector Machines* or other means [TLM05, PRH10] facilitates non-local volume classification by allowing the user to paint classes on 2D slices of the data. A probabilistic approach to clustering of a 2D transfer function domain with the help of GMMs as introduced by Wang et al. [WCZ*11] supports interactive volume rendering by proposing a classification of the domain into a set of overlapping normal distributions. Wu et al. [WQ07] provide means for feature combination in the volume data. Some of these interaction techniques involve direct editing in volume space [BKW08]. Our approach unifies key advantages of these approaches. It operates directly in 3D and does not require complex histogram interaction. It does not rely on the presence of (carefully placed) slices through the data and is robust with respect to outliers in user selection. The application of one-class classification additionally allows the *direct* specification of interesting classes leading to simplified interaction operations. This facilitates classification without making concrete a-priori assumptions about a data model and feature properties for a specific data set.

3. Localized Data Models with GMMs

In the following we detail the steps of our image-based data model estimation approach as illustrated in Figures 1 and 2.

Data Selection in the Volume As interaction with histogram space can be both unintuitive in low-dimensional spaces and infeasible in high-dimensional spaces, a direct way for local data selection is 3D interaction with the volume rendering. A selection in image space corresponds to a partial histogram selection. This selection serves as a basis for local data model estimation.

Local Data Model Estimation The selection of a subset of the histogram results in a high-dimensional point-set consisting of representatives of a data model. In terms of machine learning, this set corresponds to the training data used

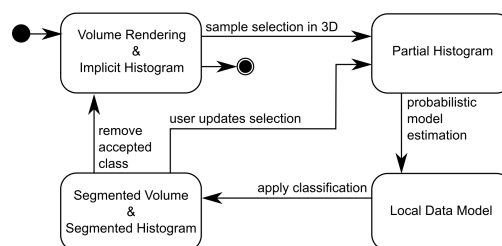


Figure 1: The user initiates automatic model estimation of the local data model by providing feature samples. This local model is used to perform classification of all remaining volume samples. Combination of classifications results in complete transfer function definition.

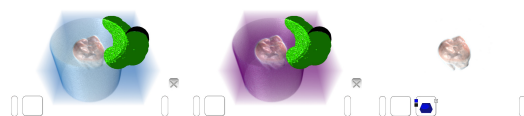


Figure 2: Left to right: After performing selection (green) in the volume, our probabilistic classifier assigns parts of the volume to the learned class (purple). The histogram and class model is shown in Figure 3. The class can be modified, discarded, or saved to the class list (rounded icons).

to construct a class model that generalizes properties of class members to the complete data set. Central requirements for modeling such a classifier in the context of this work are: Robustness to outliers to mitigate selection uncertainty, unsupervised learning, and one-class classification with appropriate generalization and fitness qualities.

Bayesian classification techniques can be adapted to satisfy these requirements in a straight-forward fashion. Since GMMs have proven to be valuable for histogram segmentation [WCS*10, WCZ*11], we employ this technique in an extended and localized fashion (see Appendix for details). Note that in this previous work, GMMs are fitted to the complete histogram and further interaction in a 2D histogram space is required to find a model that clearly emphasizes features in the volume, thus limiting histogram dimension and initial locality.

Application of GMM We apply mixed GMM estimation directly to histogram selections. The resulting set of normal distributions allows for probabilistic classification of all voxels in the data set. We perform classification in two steps. First, samples that lie within a predefined confidence interval of the extracted normal distributions are automatically classified as belonging to the class with respective probability. Because this classification is based solely on sample distributions and does not take features of the histogram into account, we perform a second step for full classification. In this second step we extend this classification to neighboring data points by taking image connectivity and histogram continuity into account. A data point j with a probability of

P_j for belonging to the current class that is not yet classified as a member is included in this classification, if all of the following conditions are fulfilled. i) Its probability P_j is significantly above zero ii) It is a direct neighbor (in image space) to a member i of the class. iii) $P_j > \delta P_i$, with $\delta < 1$.

These conditions guarantee that class membership is only extended to voxels that are spatially close to definite members both in volumetric image space and histogram space, i.e., it counteracts the GMMs' tendency to overgeneralize. Note that the last condition ensures neighborhood in the histogram by constraining the maximal probability gradient magnitude. The examples given in this paper use $\delta = 0.5$.

Modification of Classification Applying the probabilistic classifier to the histogram assigns class membership probabilities to all voxels of the data set, which can be modified by interaction with the volume, such as sample addition, until the user visually verifies the local data model. After verification, the local data model is saved to a list of valid classifiers for the data set and its members (for a given confidence value) are removed from the volume.

4. Results

We apply our techniques to three data sets that are frequently used in the volume rendering community. The data sets have different optimal histogram dimensions. The tooth data set is the most complex out of the three, where an optimal classification requires three or more dimensions in the histogram.

4.1. Interaction and Rendering

We provide the user with a spherical selection tool that moves along the surface of the (unclassified) volume. By providing a simple direct volume rendering we enable the user to create data selections for classification. Note that an online classification of voxels based on a class model that is represented by a large set of Gaussians slows down volume rendering significantly, since large numbers of Gaussians have to be evaluated [KPI*03] per sample point on the rays. To alleviate this performance problem we make use of pre-classified volume ray-casting [EKE01], i.e., each voxel is assigned class memberships during class construction.

The interaction process follows the steps illustrated in Figure 1 and shown in practice in Figure 2. In the given examples, we employ a transfer function mapping gradient magnitude to opacity and scalar values to a blue-white-red colormap. During interaction, regions within the selection sphere are highlighted, and selection is performed in voxel space, where a mask is updated locally during run-time to display selected regions of the volume. After selection, a mixture of GMMs is fitted to the selected subset of the histogram and used for voxel classification. Notice how after fitting samples of the current class are marked as classified (in purple). The user can inspect or drag and drop this class

into a class-browser for later modification. This interface is similar to work proposed by Tzeng et al. [TM04]. Editing of the selection, discarding or saving of the generated class is possible. Saved classes are shown in a class list for further interaction, such as specification of optical properties or class merging. Figure 3 shows a histogram rendering of the selection made in the Tooth example. This selection process guides local feature classification in the histogram as opposed to global fitting [WCS*10].

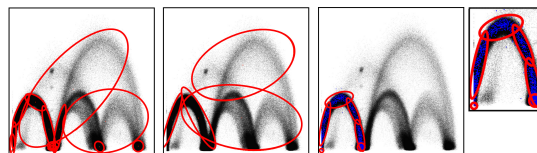


Figure 3: Global GMM fitting (c.f., [WCS*10]) (left, 14 Gaussians) produces multiple small Gaussians in high density regions. Only clipping of these regions can allow for more balanced global fitting with less Gaussians (middle, 4 Gaussians). Right: The model of an intensity-gradient selection (blue) is estimated locally as a mixture of GMMs using our technique (c.f., close-up). The GMM is used to assign class membership probabilities and together with spatial confidence growing defines the class boundaries.

4.2. Classification Results

A comparison of classifications of the tooth data using our method with automatic global GMM fitting is shown in Figure 4; the outermost class is transparent. The automatic classification employs a 2D transfer function domain to allow for the easy distinction of multiple classes. Note how our approach performs localized fitting and can produce results for 3D histograms, since no interaction in histogram space is required. Interactive classification with our approach required on average three selection iterations per class.

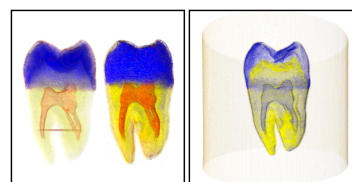


Figure 4: A classification of the tooth data. Left: Our approach (using 2D histogram on the left, 3D on the right), showing three local classes. Note how 3D classification removes an extra feature visible in the background. Right: The two meaningful classes as obtained by EM fitting of 4 Gaussians (see Figure 3) in the intensity-histogram. The latter suffers from bad classification due to automatic global fitting. Interactive adjustments to this classification are only possible for 2D histograms (see [WCS*10]).

A simpler data set, whose main classes are fully separable in 2D is given by the engine data set. Figure 5 gives an impression of the selection process along with the three major

classes found in the data set. The last data set was classified in two dimensions, revealing bones and skin (see Figure 6). Fine details are preserved by the classification techniques and selection uncertainty is mitigated as indicated by clearly segmented features with probabilistic class memberships.

The performance of interaction depends largely on computational efficiency of the model estimation procedure. The proposed mixture of GMMs generally does not achieve interactive frame rates for large numbers of data points. For the given examples, classification took between 10 and 30 seconds depending on the complexity of the point distribution, despite the use of optimizations such as localized Gaussian kernels, space subdivision, and parallelization. For an on-line local data model generation further optimizations have to be considered. It is notable that the optimal number of Gaussians per GMM was generally low (below 4) in all examples, thus allowing constriction of range search during GMM estimation to $n \in [1 \dots 3]$.

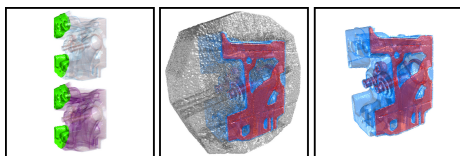


Figure 5: Classification of the engine data set. Left column: 3D interaction and resulting classification for the main engine part. Right: Three and two of the detected classes.

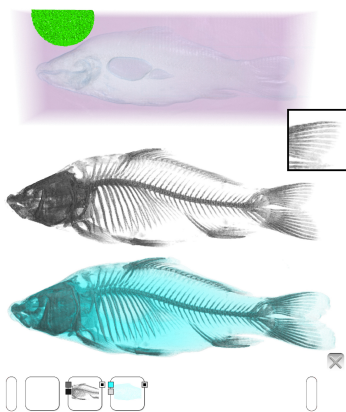


Figure 6: Classification of the fish data set into two relevant classes: Skin and bones. The first step of segmentation is commonly the removal of background material. Despite the fact that it often covers large parts of the data set, classification is fast due to very simple data distributions.

5. Conclusions and Future Work

We have introduced a concept for transfer function design that couples data-centric and interactive image-centric classification techniques. The proposed model estimation methodology was realized with the help of GMMs. While

an implementation with computationally complex estimators such as GMMs cannot perform online classification, we expect simpler methods to reach comparable results within a fraction of the time. We plan to investigate and evaluate the use of such alternative model estimators in the future.

Appendix: Mixtures of Gaussian Mixture Models

Local selections in the histogram can be interpreted as partial selections of overlapping probability density functions. Assuming a complex distribution of values, GMMs are a non-parametric method to estimate this set of distributions by fitting a number of normal distributions to the d -dimensional data. Given a parametric d -dimensional Gaussian distribution $\mathcal{N}(x; \mu, \Sigma)$ with mean $\mu \in \mathbb{R}^d$, covariance $\Sigma \in \mathbb{R}^{d \times d}$ and d -dimensional vector x , an n -component GMM is given as

$$p(x|\Theta) = \sum_i^n \omega_i \mathcal{N}(x; \mu_i, \Sigma_i). \quad (1)$$

For a specific $n \in \mathbb{N}$, estimation of the parameter array $\Theta = \{\omega_i, \mu_i, \Sigma_i\}$ is achieved by multi-dimensional Gaussian fitting [VVK03]. In our application, GMMs represent an unsupervised learning techniques suitable for model estimation. We use them to create a generative model for the locally selected data in histogram space. In practice, the number of normally distributed sources present in the data is unknown, preventing the a-priori choice of a fixed n . A solution to this problem is offered by estimating n along with Θ , effectively modeling the fitting problem as a mixture of GMMs [AAD06]. Such mixtures of GMMs eliminate the need of a-priori knowledge about the number of distributions. A non-parametric method for the computation of these mixtures performs repeated GMM fitting for a range of different n and subsequently selects the best fitting GMM. These steps are illustrated in Figure 7 (for details see [AAD06]).

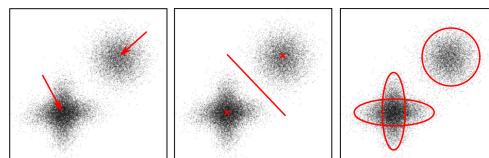


Figure 7: Steps of mixed GMM estimation. Left: Mean shift finds maxima of density (see for example [WJ94]). Middle: With the resulting maxima locations and covariance estimates, the data is clustered. Right: For every cluster, we estimate n along with Θ , resulting in sets of Gaussians.

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