

Principal Component Analysis Techniques for Visualization of Volumetric Data

Abstract

We investigate the use of Principal Component Analysis (PCA) for the visualization of 3D volumetric data. For static volume datasets, we assume, as input training samples, a set of images rendered from spherically distributed viewing positions, using a state-of-the-art volume rendering technique. We compute a high-dimensional eigenspace, that we can then use to synthesize arbitrary views of the dataset with minimal computation at run-time. Visual quality is improved by subdividing the training samples using two techniques: cell-based decomposition into equally sized spatial partitions and a more generalized variant, which we referred to as band-based PCA. The latter approach is further extended for the compression of time-varying volume data directly. This is achieved by taking, as input, full 3D volumes comprised by the time-steps of the time-varying sequence and generating an eigenspace of volumes. Results indicate that, in both cases, PCA can be used for effective compression with minimal loss of perceptual quality, and could benefit applications such as client-server visualization systems.

1. Introduction

Volumetric data comprises three-dimensional (3D) information in the form of a discretely sampled regular grid. In some cases this is obtained as a 3D stack of 2D images acquired by imaging technologies such as Magnetic Resonance Imaging (MRI), or directly generated by simulation techniques such as used in computational fluid dynamics. In recent years, there has been a trend and a demand to visualize such datasets interactively, so that viewers may peruse the dataset from different viewpoints or based on different viewing parameters. Graphics Processing Units (GPUs), which are becoming integral components in personal computers, have made it possible to generate high-fidelity interactive 3D visualizations of such data. However, the complexity of volumetric datasets in science and medicine has continued to increase to the point that, often, the dataset cannot fit in GPU memory or the processing and bandwidth overheads are too high that many of the advanced rendering techniques cannot be applied in real-time without considerable reduction of the data. At the same time, the use of portable computing devices is becoming ubiquitous, leading to a demand for visualization techniques suitable for such platforms, which are more constrained than traditional desktop graphical workstations. For instance, this has motivated the development of a number of *client-server* techniques, where a limited front-end client delivers the visualization whilst the bulk of the computational load or memory usage is devolved to a remote high-performance server or, indeed, a distributed source such as the cloud.

In this paper, we investigate the feasibility of using Principal Component Analysis (PCA) to improve the efficiency of visualizing 3D volumetric data. In particular, we are motivated by facilitating increased capacity to visualize such data without requiring

dedicated high-end computing facilities such as supercomputers. Our proposed techniques are intended to benefit visualizations on standard workstations and eventually even on minimal client devices such as mobile tablets.

Our primary contribution is a prototype approach that uses PCA to generate a high-dimensional eigenspace capturing a view-independent representation of any 3D volumetric dataset. Arbitrary views of the volume can then be reconstructed *on-demand*, at real-time rates. The efficiency of the eigenspace is improved by two adaptive decomposition mechanisms. The approach is further generalized for the compression of large highly-complex time-varying volume datasets. Experimental results indicate that our PCA-based solution can be used to generate high-quality images of 3D volumetric, whilst reducing computational complexity and data bandwidth.

2. Related Work

Volume rendering is an area of computer graphics that deals with the digital presentation of 3D volumetric data. Due to the ubiquity of such data (often referred to as *voxel* datasets), many rendering techniques have been developed over the past three decades, ranging from relatively simple slice-based techniques, that essentially blend 2D images, to highly complex 3D global illumination models. For instance, Volume Ray-casting [HKRs⁺06], is a popular technique which has become the de facto gold-standard in interactive volume rendering. Ray-casting has many advantages such as its generality, flexibility and reduced pre-processing requirement, however it is performance intensive, typically requiring a powerful graphical system with 3D texture handling support in order to achieve real-time frame rates. On the other hand, many mobile,

portable and web-based graphical systems popular in some visualization domains still have limited support for such hardware features, and thus are limited to simpler rendering techniques such as slice-based rendering.

The use of PCA for analyzing 3D objects has been well reported in the last two decades in Computer Vision and Computer Graphics. Kirby and Sirovich [KS90] proposed PCA as a holistic representation of the human face in 2D images by extracting few orthogonal dimensions which form the face-space and were called eigenfaces [TP91]. Gong et al. [GMC96] were the first to find the relationship between the distribution of samples in the eigenspace, which were called manifolds, and the actual pose in an image of a human face. Figure ?? shows manifolds distribution on the first three principal components (also called eigenfaces in this case) for different set of face poses. The use of PCA was extended using Reproducing Kernel Hilbert Spaces which non-linearly map the face-space to a much higher dimensional space (Hilbert space) [Yan02]. Knittel and Paris [KP09] employed a PCA-based technique to find initial seeds for vector quantization in image compression.

Nishino et al. [NSI99] proposed a method, called *Eigen-texture*, which creates a 3D image from a sample of range images using PCA. They found that partitioning samples into smaller cell-images improved the rendering of surface-based 3D data. Grabner et al. [GBZF03] proposed a hardware accelerated technique that uses the multiple eigenspaces method [LB00] for image-based reconstruction of a 3D polygon mesh model. To our knowledge, PCA has not yet been applied to image based-rendering of volume data, which poses additional challenges as the rendered image typically exposes interior details that need to exhibit consistent occlusion and parallax effects.

There are a number of previous reported uses of PCA-related methods in the visualization literature. For instance, Liu et al. [LWT*14] employed PCA for dynamic projections in the visualization of multivariate data. Broersen et al. [BvLH05] discussed the use of PCA techniques in the generation of transfer functions, which are used to assign optical properties such as color and opacity to attributes in volume visualization. Takemoto et al. [TNS*13] used PCA for feature space reduction to support transfer function design and exploration of volumetric microscopy data. Fout and Ma [FM07] presented a volume compression method based on transform coding using the Karhunen-Loève Transform (KLT), which is closely related to PCA.

Many remote visualisation techniques have been proposed in the scientific and medical visualization literature. The motivation for these range from facilitating collaborative multi-user systems [KBK*16], performance improvements through distributed parallel rendering [FK05], web-based visualization on browsers [PA*01], remote collaborative analysis by distant experts [SMD*13] and to achieve advanced rendering on low-spec client devices [MW08]. One strategy, in client-server volume rendering is to transmit 3D data on-demand to the client, after compression [MW08], partitioning [Bet00] or using a progressive rendering [CBPS06]. The client in all of these approaches is required to do further processing to render the data. A second alternative, such as in [EE99], is for a high-end server to remotely render the data and transmit only images to the client, which has a much reduced respon-

sibility of simply displaying the pre-rendered image. This strategy, often referred to as *Thin Client* (see Figure ??, is a popular approach for visualization on portable devices such as a mobile tablets, which may be restricted in terms of computational capacity and GPU components. In between these ends of the spectrum, some image-based approaches pre-compute intermediate 2D images that are post-processed or composited by the client before display [QT05, Bet00, TCM10]. Image-based approaches, in general, have been of interest, for improving the efficiency of volume visualization [CS98, CKT01, MPH*05]. At the cost of some additional computational load on the client, such a solution may provide improvements such as reduced latency during interaction and it is in this category that our main contributions lie.

3. Concepts

In this section we define the essential concepts and general terminology, which will be used in later sections to define our approach for interactive volume visualization using PCA.

The basic approach to PCA is as follows. Given data samples $X = [x_1 x_2 \dots x_n] \in \mathbb{R}^{d \times n}$, where each sample is in column vector format, the covariance matrix is defined as

$$C = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x})^T, \quad (1)$$

Where \bar{x} is the sample mean. After that, we can find the optimal low-dimensional bases that cover most of the data variance by extracting the most significant eigenvectors of the covariance matrix C . Eigenvectors are extracted by solving the following characteristic equation

$$(C - \lambda I)v = 0; v^T v = 1, \quad (2)$$

where $v \in \mathbb{R}^d$ is the eigenvector and λ is its corresponding eigenvalue. Eigenvalues describe the variance maintained by the corresponding eigenvectors. Hence, we are interested in the subset of eigenvectors that have the highest eigenvalues $V = [v_1 v_2 \dots v_p]$; $p \ll n$. Then we encode a given sample x using its p -dimensional projection values (referred to as *scores*) as follows

$$y = V^T x. \quad (3)$$

We can then reconstruct the sample as follows

$$x_{reconstructed} = Vy. \quad (4)$$

Since in the case of $n \ll d$, C will be of rank $n-1$ and hence there are only $n-1$ eigenvectors that can be extracted from Eq. (2) and since C is of size $d \times d$, solving Eq. (2) becomes computationally expensive. We can find such eigenvectors from the dual eigenspace by computing the $n \times n$ matrix $X^T X$ and then solving the eigenvalue problem

$$(X^T X - (n-1)\lambda I)v_{dual} = 0 \quad (5)$$

$$\Rightarrow X^T X v_{dual} = (n-1)\lambda v_{dual}; v_{dual}^T v_{dual} = 1. \quad (6)$$

Here, for simplicity, we assumed that the sample mean of X is

the zero vector. After extracting the dual eigenvectors, one can note that by multiplying each side of Eq. (6) by X , we have

$$\begin{aligned} XX^T X v_{dual} &= (n-1) \lambda X v_{dual} \\ \Rightarrow \frac{1}{n-1} XX^T (X v_{dual}) &= \lambda (X v_{dual}) \\ \Rightarrow C (X v_{dual}) &= \lambda (X v_{dual}) \\ \Rightarrow (C - \lambda I) (X v_{dual}) &= 0 \end{aligned}$$

which implies that

$$v = X v_{dual}. \quad (7)$$

In order to get the orthonormal eigenvectors, the following formula is used:

$$v_{normalized} = \frac{1}{((n-1) \text{Var}(v^T X))^{\frac{1}{4}}} v.$$

Thus, when $n \ll d$, we only need to extract the dual eigenvectors using Eq. (6) and then compute the real eigenvectors using Eq. (7). Only the first few eigenvectors $V_p = [v_1 v_2 \dots v_p]$, $p \ll n \ll d$ will be chosen to represent the eigenspace, those with larger eigenvalues. One advantage of PCA is the low computational complexity when it comes to encoding and reconstructing samples.

3.1. Normal Modes for Analysing Physical Phenomena

Any physical entity can be thought of as a network of atoms (masses) connected with each other using "spring-like" connections. Thus, the behaviour of the physical system will be governed by the vibrational motion concerted using these spring-like connections. Such a motion is due to forces that behave according to Hooke's law which assumes that the force acting at each atom k is given by

$$F_k = \Delta x_k \sum_{j=1}^n \frac{\partial^2 E}{\partial x_k \partial x_j}, \quad (8)$$

where E is the potential energy stored in the springs, Δx_k is the displacement in atom k expressed as the distance from its equilibrium position x_k . This can be written in the matrix form as follows

$$\vec{F} = H \vec{X}, \quad (9)$$

where H is the hessian matrix of potential energy. Assuming that forces are aligned with the displacements, we get

$$\lambda \vec{X} = H \vec{X} \Rightarrow (H - \lambda I) \vec{X} = 0. \quad (10)$$

By solving this eigenvalue problem we get the eigenvectors which corresponds to **Normal Modes**. These normal modes decompose the behaviour of the system into independently resonating motions. The system at any state can be expressed as a combination of such motions. Since the vibration of any atom is of sinusoidal form, this means that one can write $\vec{X}(t) = \vec{A} e^{i\omega t}$. By inserting this in the previous equations, \vec{A} gives the direction of displacement at each atom

and the corresponding eigenvalue gives the frequency at that eigenvector. The significant eigenvectors should have the lowest frequencies. Normal modes are of high importance in order to analyze the time dependent behaviour of any physical phenomena. However, using the previous technique requires a prior knowledge of the energy function which is not trivial to know in complex phenomena.

3.2. Extracting Normal Modes using PCA

Having the spatial observational measurements of a Physical phenomena stored as a time-varying volumetric data, one can consider each voxel as a single atom and the intensity value as the displacement.

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