

Chapter 18

Learning Manifolds: Design Analysis for Medical Applications

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ABSTRACT

Computer aided diagnosis is often confronted with processing and analyzing high dimensional data. One alternative to deal with such data is dimensionality reduction. This chapter focuses on manifold learning methods to create low dimensional data representations adapted to a given application. From pairwise non-linear relations between neighboring data-points, manifold learning algorithms first approximate the low dimensional manifold where data lives with a graph; then, they find a non-linear map to embed this graph into a low dimensional space. Since the explicit pairwise relations and the neighborhood system can be designed according to the application, manifold learning methods are very flexible and allow easy incorporation of domain knowledge. The authors describe different assumptions and design elements that are crucial to building successful low dimensional data representations with manifold learning for a variety of applications. In particular, they discuss examples for visualization, clustering, classification, registration, and human-motion modeling.

INTRODUCTION

Computer-aided diagnosis often implies processing large and high dimensional datasets, for instance, high-resolution volumes containing millions of voxels, or 4D videos collecting motion information over time. Visualization and analysis of such data can be very time demanding for physicians but also very computationally expensive for machines assisting diagnosis tasks. Fortunately, in many cases the relevant information for an application can be represented in lower dimensional spaces. If appropriately chosen and designed, dimensionality reduction methods will not only decrease the processing time but also facilitate any posterior analysis. Therefore, they can be of great use to a variety of CAD (Computer Aided Diagnosis) applications, ranging from general problems such as classification and visualization, to more specific ones like multi-modal registration or motion compensation. Up to recent years, dimensionality reduction in CAD has relied mainly on *linear* methods, such as Principal Component Analysis (PCA). Linear methods are however not suitable for handling non-linear complex relationships among the data samples. Non-linear approaches based on *manifold learning* are a good alternative for dimensionality reduction in such cases (Lin & Zha, 2008; Pless & Souvenir, 2009).

Established manifold learning methods like Isomap (Tenenbaum, et al., 2000), Locally Linear Embedding (LLE) (Roweis & Saul, 2000) or Laplacian Eigenmaps (Belkin & Nigoyi, 2003) are widely used in different scientific communities for data representation, dimensionality reduction, visualization, and clustering. The name “manifold” learning comes from the assumption that data-points represented in a high dimensional space lie on a low dimensional manifold; it is this manifold that the different algorithms try to approximate and represent. Several properties make manifold learning approaches very attractive, for example, flexibility, simplicity, their capability to account for non-linear data relations and their

closed form solution. The flexibility is a result of representing the data points not by their coordinates in the high dimensional space, but instead by means of relational functions between pairs of data points. These pairwise relations are determined in terms of customized similarity measures and can be non-linear functions. The core of manifold learning algorithms is independent of these measures, handing to the designer the responsibility of determining the right similarities to capture the appropriate manifold structure. Properties of manifold learning such as the flexibility and non-linearity are relevant to computer aided diagnosis, given that medical datasets tend to be high dimensional and often represent complex non-linear phenomena. Moreover, many medical datasets often verify the assumption that the data lies close to a manifold structure. For instance, the contiguous frames of a video or the slices of a volume vary smoothly; also, the continuous deformation of an organ’s shape over time can be considered to form a manifold; finally, the variations of an organ over a population can also be expected to lie on a manifold. These facts have recently raised interest in using manifold learning methods for a variety of applications, including visualization, clustering, classification, statistical shape analysis, registration, and segmentation.

A direct application of manifold learning is *visualization*. (Lim, et al., 2003) presented an early work applying manifold learning for visualizing biomedical data, where differences between bone structures were displayed in 2D by means of Isomap. Several gene expression studies (Nilsson, et al., 2004; Bartenhagen, et al., 2010) also rely on manifold learning for visualization of microarray data. Visualization of cardiac Magnetic Resonance (MR) images using Isomap was explored in (Souvenir and Pless, 2007), where images in the same breathing phase were displayed as nearby points in the low dimensional space.

Using appropriate non-linear similarity functions and neighborhood systems, manifold learning can be designed to map complex cluster

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