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Efficient isometric multi-manifold learning based on the self-organizing method

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ABSTRACT

Geodesic distance, as an essential measurement for data similarity, has been successfully used in manifold learning. However, many geodesic based isometric manifold learning algorithms, such as the isometric feature mapping (Isomap) and GeoNLM, fail to work on data that distribute on clusters or multiple manifolds. This limits their applications because practical data sets generally distribute on multiple manifolds. In this paper, we propose a new isometric multi-manifold learning method called Multi-manifold Proximity Embedding (MPE) which can be efficiently optimized using the gradient descent method or the self-organizing method. Compared with the previous methods, the proposed method has two steps which can isometrically learn data distributed on several manifolds and is more accurate in preserving both the intra-manifold and the inter-manifold geodesic distances. The effectiveness of the proposed method in recovering the nonlinear data structure and clustering is demonstrated through experiments on both synthetically and real data sets.

1. Introduction

Challenges, known as “the curse of dimensionality”, are usually confronted when scientists are conducting high dimensional data analysis. Dimensionality reduction is a promising tool to circumvent this problem. Linear dimensionality reduction methods, such as Principal Component Analysis (PCA) and Multidimensional Scaling (MDS), often fail to discover the nonlinear intrinsic structures of data. To address this issue, two Nonlinear Dimensionality Reduction (NLDR) methods, isometric feature mapping (Isomap) [32] and Local Linear Embedding (LLE) [27], were proposed in 2000. Since then, many important NLDR methods have been proposed (see, e.g. [4,31,38] for a good survey of many popular NLDR algorithms including their Matlab codes). NLDR or manifold learning has now become a fast growing research activity and proved very useful in many fields and applications, such as image retrieval [15,36], video annotation [35], clustering [10,39,42], and data visualization [3,12,21,26,34].

Most of the manifold learning algorithms implicitly assume that data points uniformly lie on a single manifold. However, in many practical applications, data points always lie on multiple clusters or multiple manifolds. For instance, in face recognition the face images of each person form its own manifold in the feature space. In motion segmentation in computer vision, moving objects trace different low-dimensional trajectories. In video sequence analysis, frames of different

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video shots form different trajectories in the low-dimensional space. Therefore, for many tasks such as multi-class recognition and data visualization, most manifold learning algorithms can only learn each class separately and fail to preserve the inter-class relationship, which restricts their application areas. To overcome this difficulty, many multi-manifold learning algorithms have been proposed, such as linear multiple learning algorithms for data classification [11,16,20], multi-manifold learning algorithms for video analysis [18,19] and for dynamic visual tracking [3,24,40], and multi-class data analysis algorithms [17,37,49]. These works have shown the advantage of multi-manifold learning algorithms over the previous manifold learning algorithms in practical applications. However, it is still a challenging problem to isometrically learn the intrinsic nonlinear data structure for multi-manifold data since it is difficult to faithfully preserve the intra- and inter-manifold distances simultaneously.

In this paper, we propose a Multi-manifold Proximity Embedding (MPE) algorithm to learn multi-manifold data in the unsupervised case. First, we propose two efficient Isometric Proximity Embedding (IPE) algorithms for data distributing on a single manifold, based on the gradient descent method and the self-organizing method. Then, a general framework is introduced for Isometric Multi-Manifold Learning (IMML), based on which the MPE algorithm is proposed for multi-manifold data. MPE is an efficient extension of IPE to multi-manifold data. The proposed MPE has two steps to realize IMML. In the first step, it discovers the data manifolds and then reduce the dimensionality of each manifold separately. Meanwhile, a skeleton representing the global structure of the whole data set is built and then mapped into the low-dimensional space. In the second step, by referring to the low-dimensional representation of the skeleton, the embedding of each manifold is relocated into a global coordinate system. Compared with the previous unsupervised IMML algorithms, our MPE algorithm is not only computationally efficient but also accurately preserves both the intra-manifold and the inter-manifold geodesic distances and therefore is more effective in recovering the nonlinear data structures and clustering.

This paper extends and improves upon our previous work [6] substantially, as indicated below.

(1) A general framework for IMML is introduced in this paper. The framework not only provides the motivation and explanations of the previous methods but can also be regarded as a general platform to design new IMML methods, such as the MPE method in this paper.
(2) With the help of the framework, the MPE method is presented in this paper which is able to preserve the geodesic distance more accurately than our previous method in [6]. Further, the MPE method is based on two efficient optimization algorithms: the gradient descent method and the self-organizing method, so it is computationally efficient and also applicable to large-scale data sets.
(3) More experiments are conducted on both synthetic and image data sets. In particular, clustering results on low-dimensional embeddings of image data are provided to show the effectiveness of the proposed method.

The rest of the paper is organized as follows. In Section 2, previous IMML algorithms are briefly reviewed. In Section 3, a general framework is first introduced for designing IMML algorithms and then used to propose a new IMML algorithm, that is, the MPE algorithm. In Section 4, the effectiveness of the proposed MPE method is demonstrated through experiments on both synthetical and image data sets. Comparisons of our MPE algorithm with several previous IMML algorithms are also made. Concluding remarks are provided in Section 5.

2. Isometric manifold learning and related IMML algorithms

Isomap was first introduced in [32] and is based on the classical MDS method. Its main idea is to preserve the geodesic distance on the data manifold in finding the low-dimensional embedding manifold. Another isometric manifold learning method, namely the GeoNLM [48], has been shown more robust to short circuit edges than Isomap. In these two methods, the geodesic distance between two data points is approximated by the shortest path on a constructed graph using Dijkstra's or Floyd–Warshall's algorithm. If the data points distribute on several clusters or manifolds, neither the k-NN method nor the ε-NN method can construct a good quality neighborhood graph. Therefore, both Isomap and GeoNLM fail to work on this kind of data, which limits their applications. Much work has been done to extend the two methods to multi-manifold learning, which will be briefly reviewed as follows.

Wu and Chan [41] proposed a split-augment approach to construct a neighborhood graph. Their method can be regarded as a variation of the k-NN method, which is simple to implement and has the same computational complexity as the k-NN method. However, since there is only one edge connecting every two graph components, the geodesics across the components are poorly approximated.

Yang [44–47] introduced four methods to construct a connected neighborhood graph: the k minimum spanning trees (k-MST) method [44], the minimum-k-spanning trees (Min-k-ST) method [45], the k-edge-connected (k-EC) method [46] and the k-vertices-connected (k-VC) method [47]. These methods have the following advantages over the k-NN method. First, the local neighborhood relationship is affected by the global distribution of the data points. This is beneficial for adaptively preserving the global geometric metrics. Secondly, these methods can guarantee that the constructed neighborhood graph is totally connected. Thirdly, compared with the k-NN method using the same neighborhood size k, the neighborhood graph constructed by Yang's methods contains more edges. These properties ensure the good quality of the neighborhood graphs. However, these methods are computationally expensive (see [50,51]).