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Manifold learning: Dimensionality reduction and high dimensional data reconstruction via dictionary learning ☆

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ABSTRACT

Nonlinear dimensionality reduction (DR) algorithms can reveal the intrinsic characteristic of the high dimensional data in a succinct way. However, most of these methods suffer from two problems. First, the incremental dimensionality reduction problem, which means the algorithms cannot compute the embedding of new added data incrementally. Second, the high dimensional data reconstruction problem, which means the algorithms cannot recover the original high dimensional data from the embeddings. Both problems limit the application of the existing DR algorithms. In this paper, a dictionary-based algorithm for manifold learning is proposed to address the problems of incremental dimensionality reduction and high dimensional data reconstruction. In this algorithm, two dictionaries are trained. One is for the manifold in the high dimensional space and the other one is for the embeddings which can be computed by any existing DR method in the low dimensional space. When new data is added, dimensionality reduction and data reconstruction can just be conducted by coding this input data over one dictionary, and then use this code to recover the output data via the other dictionary. The proposed algorithm provides a general framework for manifold learning. It can be integrated into many existing DR algorithms to make them feasible to both incremental dimensionality reduction and high dimensional data reconstruction. The algorithm is efficient due to the closed-form solution for sparse coding and dictionary updating. Furthermore, the proposed algorithm is space-saving because it only needs to store two dictionaries instead of the whole training samples. Experiments conducted on synthetic datasets and real world datasets show that, no matter for incremental dimensionality reduction or high dimensional data reconstruction, the proposed algorithm is accurate and efficient.

1. Introduction

Manifold learning has been researched intensively in recent years. It can reveal the intrinsic characteristic of the high dimensional data in a succinct way. The objective of Manifold learning is to find a description of low-dimensional structure of an unknown low dimensional manifold embedded in high dimensional ambient Euclidean space [1]. In general, manifold learning can be classified into two categories. One category is Manifold Approximation. The main idea of these Manifold Approximation method is to decompose the data manifold into small regions, each region is piecewise approximated by some geometrical structure, such as simplicial complex [1], k-means and k flats [2], etc. However, these Manifold Approximation methods do not find a low-dimensional parameterization on the Data Manifold and such parameterization is usually required in the Machine Learning/Data Mining tasks dealing with high-dimensional data. Another approach in manifold learning is to extract a low-dimensional structure from high dimensional data, which can be viewed as the problem of finding the mapping from the high dimensional data to its embedding. From this perspective, the manifold learning task involves two aspects: dimensionality reduction and high dimensional data reconstruction. Dimensionality reduction is to find the low dimensional embedding of the high dimensional data. High dimensional data reconstruction is to recover the high dimensional data from the low dimensional embedding. They are inverse problem to each other. In the past decades, many dimensionality reduction (DR) algorithms have been proposed, including linear dimensionality reduction (LDR) algorithms and nonlinear dimensionality reduction (NLDR) algorithms [3]. The typical linear methods are PCA [4–6] and MDS [7,8]. PCA computes the embedding by projecting the data to new axes on which the projected data has the maximal variances. MDS computes the low dimensional embedding by

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preserving the inner product for each pair of points. However, LDR cannot deal with the curve manifold. In such case, we need to use NLDR. As for NLDR, two pioneer works are ISOMAP [9] and LLE [10]. ISOMAP captures the global geometric structure by computing the geodesic distance for each pair of points on the manifold and then applies MDS to find the low dimensional embedding. LLE constructs a local geometric structure that is invariant to translation, scaling and orthogonal transformation for each point on the manifold, and computes the embedding by preserving these local geometric structures. The following research works on nonlinear dimensionality reduction include LTSA [11], HLLE [12], LE [13,14], LPP [15], MVU [16], LLC [17], MLE [18] and many other algorithms [19–23]. Though many NLDR algorithms have been proposed, most of them suffer from two problems. One is that many of them have complexity as $O(N^2)$ or even $O(N^3)$, where N is the number of samples. This high computational cost makes it difficult to deal with the large-scale task in the real world. The other one is that most of these algorithms cannot perform dimensionality reduction in an incremental way. This means when a new data point is added, to find its embedding, we have to use the whole updated dataset to compute all the embedding again in a batch way, which is time consuming. To overcome this problem, the incremental algorithms for ISOMAP, LLE, LTSA, LE and HLLE have been proposed in recent years [24–28]. Though these methods can reduce the computational complexity, they still need to compute all the embedding again when a new data point is given. Furthermore, these incremental algorithms are closely related to the corresponding DR algorithms, which means that the incremental algorithm of one DR algorithm cannot be applied to other DR algorithms. The generalization is limited. Therefore, it is meaningful to develop a general algorithm that can be integrated into the existing DR algorithms to make them gain the ability to perform incremental dimensionality reduction and deal with large scale problem.

While dimensionality reduction problem has been researched intensively, its inverse problem (i.e. high dimensional data reconstruction) has not been well studied. Most existing DR algorithms are only interested in how to reduce the dimensionality of the high dimensional data but seldom involve with how to recover the high dimensional data from the embedding. In some applications, data reconstruction is also useful. As we will show in the following experiments, the image decompression, expression synthesis and pose synthesis can be all converted to the data reconstruction problem. Though some of the DR algorithms provide reconstruction algorithms, such as LTSA, LLC and MLE, the reconstruction algorithms are also close related to the DR algorithms. In other words, the reconstruction algorithm for one DR algorithm is not applicable to the other DR algorithms. Therefore, it is useful to develop a general data reconstruction algorithm that can be integrated into the existing DR algorithms to make them have the ability to perform data reconstruction.

To solve these problems mentioned above, this paper proposes a novel and practical dictionary learning-based algorithm that can be used for both dimensionality reduction and high dimensional data reconstruction. Dictionary learning has been widely studied and proven to be an effective method in image processing and pattern classification [29–34]. In the past few years, many dictionary learning algorithms have been proposed for different purposes [35–38]. However, its application in manifold learning is seldom reported. Though recently some researchers have proposed a dictionary-based algorithm to perform NLDR [39], they also do not consider the problem of original high dimensional data reconstruction. In this paper, we show that the manifold learning problem can be converted to the dictionary learning problem. In the proposed algorithm, we train two dictionaries. One is for the manifold in the high dimensional space and the other is for the embedding in the low dimensional space. With these two dictionaries, the high dimensional data and its embedding can be linked by the shared code on these two dictionaries. For a new input sample, we compute its coding over one dictionary, and then use this coding to compute the output via the other dictionary. Experiments show that our algorithm has the following four advantages: first, since the coding has an analytic solution, dimensionality reduction can be performed efficiently, and therefore the proposed algorithm can be used in large-scale problem. Second, the proposed algorithm can be integrated into many DR algorithms to make them have the extra ability to perform incremental dimensionality reduction. Third, the proposed algorithm presents a general method for high dimensional data reconstruction. It can be integrated into many existing DR algorithms to make them have the ability to perform high dimensional data reconstruction. Fourth, the proposed algorithm has low space complexity. No matter for dimensionality reduction or data reconstruction, what we need to store are two dictionaries, which need much less storage space than the training samples do.

The rest of the paper is organized as follows: In Section 2, a simple example is presented to illustrate the motivation of our algorithm. In Section 3, the details of our dictionary-based algorithm are given. In Section 4, experiments on synthetic datasets and real world datasets are conducted to evaluate the performance of the proposed algorithm. Finally, in Section 5, some issues related to the proposed algorithm are discussed.

2. Motivation

Before we give the details of our algorithm, we first use a simple example to illustrate the idea of our algorithm. In this example, the high dimensional data are sampled from the Swiss-roll. Swiss-roll is a famous dataset in manifold learning. It resides in the three-dimensional space, but its intrinsic dimensionality is two. The blue points in Fig. 1(a) are the samples randomly drawn from Swiss-roll, and the blue points in Fig. 1(b) are the corresponding embeddings of these samples. Our algorithm is motivated by LLE [10]. Indeed, many general techniques for non-linear dimensionality reduction have been developed that rely on the *manifold hypothesis* which states that the high dimensional data manifold lies on or near a smooth non-linear manifold of lower dimensionality. Under the *manifold assumption*, previous studies focus on using differential operators to construct a regularization functional on the manifold. These methods can be roughly classified into three categories: Laplacian regularization, Hessian regularization [40,41], and parallel field regularization [42]. LLE [10] can be viewed as Laplacian operator based methods which mainly consider the local neighborhood structure of the manifold, which use the graph Laplacian to measure the smoothness of the learned function on the manifold. In LLE, the high dimensional data point x_i is first approximated by the linear combination of its nearest neighbors. That is $x_i \approx \sum_{j=1}^{K} a_j x_{ij}$, where $x_{ij}, j = 1, \dots, K$ are the K nearest neighbors of x_i and $a_j, j = 1, \dots, K$ are the combination coefficients satisfying $\sum_{j=1}^{K} a_j = 1$. LLE first computes the optimal a_j by minimizing $\|x_i - \sum_{j=1}^{K} a_j x_{ij}\|^2$ with regard to a_j, and then keeps a_j unchanged to minimize $\|y_i - \sum_{j=1}^{K} a_j y_{ij}\|^2$ with regard to y and y_{ij}. The optimal y and y_{ij} are the embedding of x and x_{ij}, respectively. The basic idea of LLE is that, in a small neighborhood of x_i, the optimal combination coefficients $a_j, j = 1, \dots, K$, for $\|x_i - \sum_{j=1}^{K} a_j x_{ij}\|^2$ are invariant to translation, scaling and rotation of the data, and therefore the combination coefficients for y_i are also the same as x_i's. It motivates us that the combination coefficients can be used as a link between the high dimensional data and their embedding. Based on this observation, we propose a