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Locality-preserving low-rank representation for graph construction from nonlinear manifolds

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ABSTRACT

Building a good graph to represent data structure is important in many computer vision and machine learning tasks such as recognition and clustering. This paper proposes a novel method to learn an undirected graph from a mixture of nonlinear manifolds via Locality-Preserving Low-Rank Representation (L^2R^2), which extents the original LRR model from linear subspaces to nonlinear manifolds. By enforcing a locality-preserving sparsity constraint to the LRR model, L^2R^2 guarantees its linear representation to be nonzero only in a local neighborhood of the data point, and thus preserves the intrinsic geometric structure of the manifolds. Its numerical solution results in a constrained convex optimization problem with linear constraints. We further apply a linearized alternating direction method to solve the problem. We have conducted extensive experiments to benchmark its performance against six state-of-the-art algorithms. Using nonlinear manifold clustering and semi-supervised classification on images as examples, the proposed method significantly outperforms the existing methods, and is also robust to moderate data noise and outliers.

1. Introduction

Graph-based methods have attracted a lot of attention over the last decade in the field of computer vision and machine learning. Various graph-based algorithms have been successfully applied in diverse scenarios, such as image segmentation [1–3], semi-supervised learning [4], and dimensionality reduction [5,6]. Their core idea is to learn a discriminative graph to characterize the relationship among the data samples. However, how to learn a good graph to accurately capture the underlying structure from the observed data is still a challenging problem. In this paper, we propose a novel method to address the graph construction problem for nonlinear manifolds based on some emerging tools in low-rank representation and sparse optimization.

Conceptually, a good graph should reveal the true intrinsic complexity or dimensionality of the data points (say through local linear relations), and also capture certain global structures of the data as a whole (i.e. multiple clusters, subspaces, or manifolds). Traditional methods, such as *k-nearest neighbors* and *Locally Linear Embedding* (LLE) [7,8], mainly rely on pair-wise Euclidean distances to build a graph by a family of overlapping local patches. Since pair-wise distances only characterize the local geometry of these patches by linearly reconstructing each data point from its neighbors, these graphs can only capture local structures, and are very sensitive to local data noise and errors as well. Moreover, traditional methods only work well for a single manifold, and often fail when data points arise from multiple manifolds.

Most recently, in order to capture the global structure of the data, several methods [9–13] have been proposed to construct a sparse and block-diagonal graph with new mathematical tools (such as *sparse representation* [14] and *Low-Rank Representation* [12]) from high-dimensional statistics and covex optimization. Different from traditional methods, these methods represent each datum as a linear combination of all the remaining samples (such as in [9,10]) or all the whole data (such as in [11–13]). Here, we call them *Representation-based methods*. By solving a high-dimensional convex optimization problem, these methods automatically select the most informative neighbors for each datum, and

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simultaneously obtain the graph adjacency structure and graph weights in nearly a parameter-free way. Benefitting from the new mathematical tools, these methods are able to generate a block-diagonal graph, and are robust to data noise. However, the block-diagonal structures obtained by these methods are often fragile, because they hold the hypothesis that the manifold can be embedded linearly or almost linearly in the ambient space. Unfortunately, in real applications, this hypothesis may not be always true. It has been proven that many high-dimensional data usually exhibit significant nonlinear structure, where these representation-based methods often fail to deliver satisfactory performance. As a result, the block-diagonal structures cannot be enforced strictly in this case.

In fact, studies on manifold learning have shown that, to deal with data sampled from nonlinear manifolds [15–17], one has to exploit the local geometrical structure of manifold, or use a nonlinear mapping to "flatten" the data (such as kernel methods [18,19]). In order to preserve the local geometrical structure embedded in high-dimensional space, some graph regularizers are readily imposed on the linear combination representation of the data. For example, Zheng et al. proposed a method called *Low-Rank Representation with Local Constraint* (LRRLC) [15] by incorporating the so-called *local consistency assumption* into the original *Low-Rank Representation* (LRR) model, with the hope that if two samples are close in the intrinsic geometry of the data distribution, they will have a large similarity coefficient. LRRLC introduced a weighted sparsity term (i.e. graph regularization term) with data-dependent weights into the original LRR model. The weights changed with the distance between samples. However, the graph regularization term could not guarantee that close samples would have large similarity coefficient. It only enforced the coefficients between faraway points to be small. Essentially, the LRRLC model only used the relationship among points to re-weight the linear representation.

Our goal is to preserve both the global structure *and* the local structure in our constructed graph. To capture the global structure, the linear representation Z should be block diagonal, which means that the coefficient Z_{ij} should be zero if data point x_i and x_j are not in the same cluster.[1] Since the local consistency assumption only encourages the coefficients between close samples to be nonzero, it will not necessarily lead to being block diagonal. On the contrary, the LRRLC model often fails to accurately represent the geometric structure of manifolds because of two drawbacks. First, LRRLC directly uses affine subspaces to find neighborhoods of points, and thus are likely to select faraway points as neighbors. This may cause a coefficient between two faraway points to be nonzero, even if they belong to different manifolds or are well separated by other points on the same manifold. Second, LRRLC uses the non-negativity constraint to define neighborhood for every point. When a point is on a boundary, this constraint may choose points from other manifold/subspace as its neighbors, or the boundary point will be isolated. These two drawbacks often violate the block diagonalization of its solution in the LRRLC model. As a result, the LRRLC model often obtains a dense graph that negatively affects its performance.

1.1. Contributions

Inspired by the above insights, we propose to extend the LRR model to construct an informative graph called *Locality-Preserving Low-Rank Representation Graph* (L^2R^2-graph). Specially, given a set of data points, we represent each data point as a linear combination of all the other points. For each point, we determine its neighbors according to the pair-wise distance. By restricting the coefficient Z_{ij} for non-neighbors to be zero and imposing the affine constraint, we approximate the nonlinear manifold by a collection of affine subspaces. Since we require that data vector on the same affine subspace can be clustered in the same cluster, we require that the coefficient vectors of all data points collectively form a low-rank matrix. By imposing the low-rank constraint, the L^2R^2-graph can better capture the global cluster or subspace structures of the whole data, and is more robust to noise and outliers.

It is worthwhile to highlight several advantages of L^2R^2-graph over the existing works:

1. Compared with traditional methods, since L^2R^2-graph imposes the low-rank constraint, it can better capture the global structure. Moreover, as shown in later experiments, though L^2R^2-graph uses pair-wise distance to define the graph adjacent structure, it is insensitive to the global parameters, while traditional methods are more sensitive to the global parameters.
2. Compared with other representation-based methods based on the hypothesis of linear subspaces, L^2R^2-graph explicitly considers the local structure of manifolds, and preserve it during graph construction. Such local structure preservation makes the learned L^2R^2-graph more sparse than these representation-based methods.
3. Compared with LRRLC-graph [15], L^2R^2-graph can better preserve the geometric structure of manifolds. In LRRLC-graph, the local structure is used to re-weight the linear combination coefficients, which compromises the block diagonality assumption of the representation. While in L^2R^2-graph, the local structure is used to define the neighborhood of each point. Since restricting the coefficient Z_{ij} for non-neighbors to be zero may not affect the block diagonality of the representation Z, the resulting Z could still be block diagonal in ideal cases.

We conduct extensive experiments on simulation data and public databases for two typical tasks, namely nonlinear manifolds clustering and semi-supervised classification. The experimental results clearly demonstrate that the L^2R^2-graph can significantly improve the learning performance, and is more informative and discriminative than other graphs constructed by conventional methods.

The remainder of this paper is organized as follows. In Section 2, we give the details of how to construct a locality-preserving low-rank graph. Our experiments and analysis are presented in Section 3. Finally, Section 4 concludes our paper.

2. Graph building via locality-preserving low-rank representation

2.1. Low-rank representation: an overview

Low-Rank Representation (LRR) was proposed to segment data drawn from a union of multiple linear (or affine) subspaces. Given a set of sufficiently dense data vectors $X=[\boldsymbol{x}_1,\boldsymbol{x}_2,\ldots,\boldsymbol{x}_n]\in\mathbb{R}^{d\times n}$ (each column is a sample) drawn from a union of k subspaces, LRR seeks the lowest-rank representation that represent all the vectors as the linear combination of the data themselves, and solves the following convex optimization problem:

$$\begin{aligned}&\min_{Z,E}\quad \|Z\|_*+\lambda\|E\|_{2,1},\\ &\text{s.t.}\quad X=XZ+E,\end{aligned}\tag{1}$$

[1] Note that it is a misconception for Z to be block diagonal that Z_{ij} should be nonzero if x_i and x_j are in the same cluster.