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Improved hypergraph regularized Nonnegative Matrix Factorization with sparse representation

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ABSTRACT

As a commonly used data representation technique, Nonnegative Matrix Factorization (NMF) has received extensive attentions in the pattern recognition and machine learning communities over decades, since its working mechanism is in accordance with the way how the human brain recognizes objects. Inspired by the remarkable successes of manifold learning, more and more researchers attempt to incorporate the manifold learning into NMF for finding a compact representation,which uncovers the hidden semantics and respects the intrinsic geometric structure simultaneously. Graph regularized Nonnegative Matrix Factorization (GNMF) is one of the representative approaches in this category. The core of such approach is the graph, since a good graph can accurately reveal the relations of samples which benefits the data geometric structure depiction. In this paper, we leverage the sparse representation to construct a sparse hypergraph for better capturing the manifold structure of data, and then impose the sparse hypergraph as a regularization to the NMF framework to present a novel GNMF algorithm called Sparse Hypergraph regularized Nonnegative Matrix Factorization (SHNMF). Since the sparse hypergraph inherits the merits of both the sparse representation and the hypergraph model, SHNMF enjoys more robustness and can better exploit the high-order discriminant manifold information for data representation. We apply our work to address the image clustering issue for evaluation. The experimental results on five popular image databases show the promising performances of the proposed approach in comparison with the state-of-the-art NMF algorithms.

1. Introduction

Nonnegative Matrix Factorization (NMF) is a considerable multivariate analysis technique for data analysis [13,16,26]. It learns a part-based representation of the data via finding two nonnegative matrices whose product provides a good approximation to the original matrix. In NMF, the nonnegative constraints lead to a parts-based representation because they allow only additive, not subtractive, combinations. And such way is in accordance with the recognition way of the human brain [3,13]. Due to its good psychological and physiological interpretation, NMF has been in vogue for decades and successfully applied to a wide range of domains such as computer vision, machine learning and pattern recognition [15,17,22,30,33,36].

Recently, many studies indicate that the high-dimensional data actually resides on a low-dimensional manifold and such intrinsic geometric structure of data is very useful for discriminating data [2,23]. Over decades, extensive classical manifold learning approaches have been presented, such as Locally Linear Embedding (LLE) [23], Laplacian Eigenmapping (LE) [2] and Neighborhood Preserving Embedding(NPE) [8]. Graph learning is a popular technique for manifold learning. In graph learning, the manifold learning issue is considered as a graph cut issue [27]. The core of graph learning approaches is graph which encodes the relations of samples. During the graph partition, such relations of samples should be preserved as more as possible [2,9]. And then the manifold of data can be well kept.

In the last decade, some researchers are aware of the importance of manifold information and try to incorporate such desirable property into NMF [3,7,29–31,36,37]. Graph regularized Nonnegative Matrix Factorization (GNMF) should be one of the representative approaches in this category [3]. In GNMF, a graph is lever-

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aged to depict the neighborhood relation of data, and then introduced to NMF as a graph regularization for considering the local geometric structures preservation during the matrix factorization. The graph construction is very crucial for GNMF. Since the graph used in GNMF is the common graph whose edge only can connect two vertices, GNMF can only capture the simple pairwise relation of data and clearly neglect the high-order relation among the samples. To address this issue, Zeng et al.[36] presented the Hypergraph regularized Nonnegative Matrix Factorization (HNMF) for image clustering via using hypergraph instead of graph to depict the data structure. The reason why HNMF can address such problem is that hypergraph is a generalization of graph and its edge can connect any number of vertices [38]. In order to better address the hyperspectral unmixing task, Wang et al.[31] introduces a conventional hypergraph regularization to $L_{1/2}$-NMF for better exploiting spectral-spatial joint structure of hypespectral image. Generally speaking, a graph can only depict one relation (or measure) of samples. However, in most of time, it is very hard to pick up a suitable data relation to address different issues. Wang et al.[30] alleviated this problem by presenting Multiple Graph regularized Nonnegative Matrix Factorization (MultiGrNMF). In MultiGrNMF, multiple graphs, which encode different data relations, are combined as a combative graph regularization for constraining NMF. These graphs are deemed as a series of initial guesses of the optimal graph Laplacian. And, finally, the optimal combination of graphs can be conditionally learned by ensemble manifold regularization technique [6]. The main drawback of MultiGrNMF over other GNMF algorithms is that it is very time consuming to construct multiple graphs. Moreover, from the perspective of graph embedding [28], many constrained NMF algorithms actually can be formulated as a specific GNMF algorithm [14,24,32].

In HNMF or GNMF algorithms, a good graph (or hypergraph) is an important key towards to the success, since a high-quality graph can well reveal the real relations among samples and these relations are the crucial cues for data analysis. In GNMF or graph learning approaches, the k-nearest neighbor is the most commonly adopted method for graph (or hypergraph) construction. However, many studies have shown such graph construction fashion is sensitive to noise and often cannot correctly reflect the real relation of samples. Recently, motivated by the advancements of Sparse Representation (SR) [12], some researchers have attempted to leverage sparse representation for constructing the high quality graph. The sparse representation-based graph is often called sparse graph or L_1-graph. Since it inherits the merits of SR which is very discriminative and robust to noise, the sparse graph works have already achieved remarkable success in many domains [4,11]. We believe the success of sparse graph can be also applied to HMMF and GNMF. So, in this paper, we focus on applying sparse representation to construct a more robust and discriminative hypergraph for constraining NMF. We call such novel NMF algorithm Sparse Hypergraph regularized Nonnegative Matrix Factorization (SHNMF). Since the sparse representation-based hypergraph inherits the merits from both the hypergraph and the sparse representation, SHNMF enjoys more desirable properties and has a much better performance over the conventional GNMF and HNMF algorithms. Moreover, SHNMF is different to the other conventional sparse GNMF, such as Hypergraph regularized $L_{1/2}$-NMF [31] or Graph regularized $L_{1/2}$-NMF algorithms [18], which emphasize on the sparsity of loading matrix. However, SHNMF emphasizes on the sparsity of the hypergraph whose main idea is to leverage the sparse representation to construct a high-quality hypergraph for regularizing NMF. We adopt five popular image databases to evaluate the data representational power of SHNMF. The experimental results demonstrate the superiority of SHNMF in comparison with the state-of-the-art NMF algorithms.

The rest of paper is organized as follows: the background knowledge and some basic notations are introduced in Section 2. Section 3 presents the methodology of our work; The experimental results are analyzed and discussed in Section 4; the conclusion is finally summarized in Section 5.

2. Preliminaries

Let us denote a set of n samples as a $l \times n$-dimensional matrix $X = [x_1, \cdots, x_n]$ where x_i is the ith sample which is corresponding to the ith column of matrix X. In the matrix factorization task, the sample matrix can be approximately factorized as $X \approx WU^T$ where the $l \times m$-dimensional matrix $W = [w_1, \cdots, w_m]$, $m \leq l$ is denoted as the bases (the basis vectors) while the $n \times m$-dimensional matrix $U = [u_1, \cdots, u_n]$ is denoted as its corresponding coefficients (loadings). For each sample, we have $x_i \approx Wu_i^T$. Clearly, such equation $X \approx WU^T$ represents the reconstruction process of sample matrix via using the bases and loadings. Its reverse process can be done as $u_i^T = W^- x_i$.

2.1. Nonnegative Matrix Factorization (NMF)

Compared to the other matrix factorization techniques, Nonnegative Matrix Factorization (NMF) imposes the non-negativity constraints $W, U \geq 0$ to ensure that all entries of W and U are nonnegative. Consequently, NMF only allows non-subtractive combinations. There are two cost functions can be defined to find an approximate factorization $X \approx WU^T$. The first one bases on the Euclidean distance and the second one bases on divergence. In this paper, we only introduce the Euclidean distance based version and the divergence based version can be referenced from their original papers. So, the NMF problem can be finally formulated as a following optimization problem:

$$\hat{W} = \underset{W,U}{\operatorname{argmin}} ||X - WU^T||^2, \quad s.t \quad W, U \geq 0 \tag{1}$$

The above problem can be solved by using multiplicative updating rules [26]. Furthermore, an additional constraint $\sum_i w_{ij} = 1$ is always imposed for stabilizing the computation, but this is not necessary.

2.2. Hypergraph

As a generalization of graph, hypergraph is an important tool for data representation. It depicts the structure of data via measuring the similarity between groups of points [10,38]. The main difference between hypergraph and graph is that the edge of hypergraph can own any number of vertices while the one of graph can only connect two vertices. The edge of hypergraph is often called hyperedge. When the length of hyperedge is equal to two, the hypergraph is exactly equivalent to a common graph. Due to the aforementioned property of hyperedge, hypergraph enjoys a higher flexility for depicting the high-order relation. In the real world, the relations among data should be more complex than the simple pairwise and naively squeezing such complex relations into pairwise ones will inevitably lead to loss of information which can be expected valuable for learning tasks. Take the article coauthor relationship as an example, an article is often corresponding to several authors. And, apparently, a common graph cannot intuitively describe such one to n high-order relation. Even in GNMF algorithms, some works also empirically validate this argument. In the experiments of Zeng et al. [36], Hypergraph regularized Nonnegative Matrix Factorization (HNMF) which utilizes hypergraph instead graph for considering the high-order relations among samples achieve a better performance in comparison with GNMF [3].

Here, we introduce some basic concepts and notations of hypergraph. Let $G(V, E)$ denote a hypergraph with vertex set $V =$