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Structure constrained nonnegative matrix factorization for pattern clustering and classification

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ABSTRACT

Decomposing data into a small number of essential components is usually an efficient strategy for data exploration, analysis and interpretation. Various workhorse methods such as principal component analysis (PCA) and nonnegative matrix factorization (NMF) have been developed along this line of ideas. These methods impose different constraints (e.g., orthogonality for PCA) to obtain compact or physically meaningful bases. However, it is more natural to learn the constraints directly from data and use them to guide the decomposition procedure. Also, existing methods mainly focus on inter-sample information and the intra-sample structure information has rarely been explored. We propose a novel method, called structure constraint nonnegative matrix factorization (SCNMF), which makes use of the intra-sample structures to facilitate the decomposition process. SCNMF mimics the recognition mechanism of the human brain to extract structure information, and has several attractive properties like always generating orthogonal bases. For concept proof and illustration purpose, human face images are the primary data used in our experiment studies, and the results suggest a superior performance of SCNMF over other representative decomposition algorithms. To illustrate the generality of the proposed method, we also show one example of the application of SCNMF in supervised learning of electrocorticography data.

1. Introduction

Complex data can be decomposed into (maybe just a small number of) essential components for efficient data representation and analysis. A representative example is human face images, which consist of only a few parts like eyes, mouth and nose. These parts have their own geometric structures, which carry important information for characterizing the similarity or distance between different image samples. Interestingly, previous psychological and physiological studies have also provided evidence for a part-based recognition mechanism in the human brain [2]. Therefore, the identification of *intra-sample components* and the usage of their *structure information* can be of significant interest and importance in confronting the need for complex data analysis. For concept proof and illustration purpose, we primarily use face images as data example unless explicitly stated otherwise (for different data types, see the electrocorticography data example in Section 4); also, the two words component and part are used interchangeably hereafter.

Along the line of the decomposition idea, a variety of methods have been developed to transform raw data into a (weighted) combination of a set of components. For instance, principal component analysis (PCA) [4], independent component analysis (ICA) [5], nonnegative matrix factorization (NMF) [6–8] and many of their variants [1,3,7] have been developed in previous studies. Among all these methods, the NMF-family approaches are attractive since physically meaningful parts can be obtained after matrix factorization [9]. However, there are three important problems have not been sufficiently addressed. First, to the best knowledge of authors, neither NMF nor other existing matrix factorization methods explicitly take the intra-sample components and their structure information into consideration. In addition, although prior knowledge of sample labels has been considered in methods like local linear embedding [10] and locality preserving projections [11], such information is inter-sample correlation and the intra-sample information does not receive sufficient attention it deserves. Therefore, it is still possible to develop more accurate learning algorithms if one can incorporate both inter- and intra-sample information into a learning procedure. Second, for existing NMF method and its variants, there is no guarantee that these methods will always produce spatially aggregated and non-overlapping parts [9], which makes the results less intuitive and interpretable. Efforts have been made to improve the NMF-family methods to this end, e.g., by

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imposing sparsity constraint [12] or inter-sample locality restriction [1]; however, such strategies may fail due to neglecting the intra-sample structure information. For illustration purpose, we show some example results from previous studies in Fig. 1. More specifically, Fig. 1(a) presents the results produced by the NMF and GNMF (Graph Regularized NMF) methods on the PIE dataset [1], and Fig. 1 (b) shows the face bases of the ORL dataset obtained by the NMF and CNMF (Constrained NMF) methods [3]. One can conclude from Fig. 1 that many of the results are not separated parts but whole faces, especially those in Fig. 1(b). Explicitly using the component structure information as constraints in the NMF-family algorithms can generate non-overlapping parts, which is proposed and investigated in this study. Third, another major concern of the NMF-family methods is how to determine the dimension (that is, the number of columns) of the basis matrix, which is usually chosen empirically without rational explanation [13]. Note that if an algorithm can decompose images into non-overlapping parts, it is natural to choose the number of parts as the number of the columns of the basis matrix because these columns are now orthogonal to each other. A few previous studies have also attempted to obtain orthogonal bases, however, at the price of compromising the non-negativity constraint and thus may not be applicable to certain problems that have a strict requirement for non-negativity [7].

To address the problems above, a structure constrained nonnegative matrix factorization (SCNMF) method is proposed in this study. Inspired by the recognition mechanism of the human brain [14,15], the intra-sample structure information is extracted from an average representation (inter-sample information) of multiple samples. The obtained structure information is then explicitly imposed as constraints on the matrix decomposition procedure. This approach turns out to be able to obtain non-overlapping parts, and have a superior performance over other representative decomposition methods.

It is worthwhile to highlight the major contributions of this paper.

1. The recognition mechanism of the human brain based on average representation is mimicked to extract the intra-sample structure constraint, which turns out to be an effective strategy according to our experiment results;
2. To the best knowledge of authors, the intra-sample structure information mined from a population of samples has rarely been explicitly incorporated into an NMF learning procedure, which is addressed for the first time in this study;
3. The proposed SCNMF method provides a natural way to determine the basis matrix dimension, and the obtained bases (columns of the basis matrix) are guaranteed to be orthogonal.

The rest of the paper is organized as follows: in Section 2 the related works are reviewed; the SCNMF method is described and theoretically justified in Section 3; experiment results are presented and discussed in Section 4; finally, the conclusions and potential future work are discussed in Section 5.

2. Related works

2.1. Structure information

Here structure information refers to spatial or geometrical patterns of data. With the increase of data complexity nowadays, the development of novel methods to efficiently identify and use the structure information embedded in data is becoming more and more important. Existing prevailing approaches like multidimensional scaling [16], isomap [17], locally linear embedding [10], and locality preserving projections [11] mainly focus on preserving

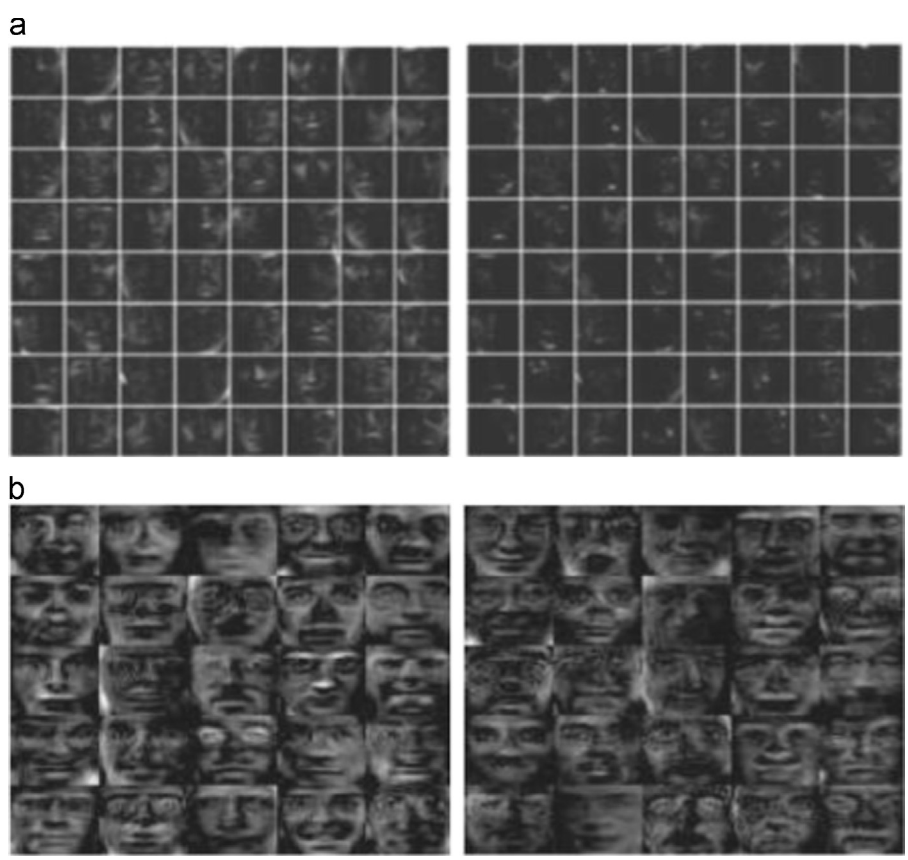

Fig. 1. Parts obtained by NMF and its variants. (a) Results obtained by NMF (left) and GNMF (right) on the PIE dataset (reprinted from [1]). (b) Results obtained by NMF (left) and CNMF (right) on the ORL dataset (reprinted from [3]).