Joint NMF for Identification of Shared Features in Datasets and a Dataset Distance Measure

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Abstract—In this paper, we derive a new method for determining shared features of datasets by employing joint non-negative matrix factorization and analyzing the resulting factorizations. Our approach uses the joint factorization of two dataset matrices $X_1, X_2$ into non-negative matrices $X_1 = AS_1, X_2 = AS_2$ to derive a similarity measure that determines how well a shared basis for $X_1, X_2$ approximates each dataset. We also propose a dataset distance measure built upon this method and the learned factorization. Our method is able to successfully identify differences in structure in both image and text datasets. Potential applications include classification, detecting plagiarism or other manipulation, and learning relationships between data sets.

Index Terms—nonnegative matrix factorization, topic modeling, dataset distance

I. INTRODUCTION

The central problem in comparing datasets is to identify fundamental similar features in the underlying structures. In image datasets, for example, this feature might point out particular structures in the image. In a document dataset, this might be a topic discussed in one data set that is not relevant in the other data set. A number of similarity and distance metrics exist for comparing data sets. McCrae et al. [1] evaluate link discovery techniques for measuring semantic textual similarity. Shahnaz et al. [2] measures the similarity between two clusters by measuring their overlap in the data set. Ben-David et al. [3] and Mansour et al. [4] developed measures to predict how well a machine learning model will perform if the source and target domains are not the same. These measures predict better performance when the source and target domains are more similar. The relatively recent work of Alvarez-Melis and Fusi [5] propose a dataset distance metric built upon an optimal transport framework.

Nonnegative matrix factorization (NMF) is a useful tool for interpretable dimension reduction. Many types of data, including documents and images, can be represented by non-negative matrices, making NMF a widely applicable method for data analysis [6]. Rad et al. [7] uses a multi-view NMF implementation to factor an image into basis vectors that are then used to generate image annotations. NMF has also been used in the creation of data set similarity metrics: Shahnaz et al. [2] clusters semantic features or topics in document data and uses NMF to preserve nonnegativity. Liu et al. [8] introduces a multi-view clustering approach based on NMF.

Joint non-negative matrix factorization (jNMF) allows for joint factorization of two data sets with a common basis [9], [10]. Additionally, jNMF for topic modeling has been used to identify similarities across data sets. Kim et al. [9] proposes a jNMF method for identifying both common and distinct topics among document data sets.

In this paper, we propose a new method for evaluating similarity between a pair of distinct data sets. This method analyzes the outputs of jNMF and measure the extent to which the basis vectors contributes to each data set. In our method, we first run jNMF on the two data sets and then compare the resulting factorizations. Additionally, we use this learned information to propose a dataset distance measure.

In Section II, we give a brief overview of NMF and jNMF. In Section III, we propose a method for determining shared features in data sets, a distance measure based on this method, and we list some desirable properties of a distance measure. In Section IV, we present examples of this method applied to real world data and experimentally verify our desired properties.

II. OVERVIEW OF NMF AND JNMF

Given a nonnegative $m \times n$ matrix $X$, the goal of non-negative matrix factorization (NMF) is to find nonnegative matrices $A$ and $S$ such that

$$X \approx AS$$
where $A$ is $m \times k$ and $S$ is $k \times n$. One typically chooses $k$ such that $AS$ is a low rank approximation of $X$; there are many heuristics and considerations for choosing model rank $k$, which are beyond the scope of this paper. NMF produces $A$ and $S$ by attempting to minimize the non-convex objective function,

$$\|X - AS\|_F^2 = \sum_{ij} (X_{ij} - (AS)_{ij})^2.$$ 

NMF models can be trained with many methods. One of the most popular methods is multiplicative updates, which is a variant of gradient descent that ensures entrywise non-negativity in the factors [11]. We typically interpret columns of $A$ as a set of “basis” vectors and the $i$th column of $S$ as the coefficients of the conic combination of those basis vectors that approximates the $i$th data point. We do not focus on how basis vectors are combined to create individual elements, but instead analyze the rows of $S$ to measure the contribution of each basis vector to the entire data set.

Joint NMF (jNMF) finds low-rank, non-negative approximations for two matrices, $X$ and $Y$, that share a common factor matrix. When applied to supervised NMF, jNMF typically factors $X$ (the data) and $Y$ (e.g., class labels) as $X \approx A_1S$ and $Y \approx A_2S$, such that the factor $S$ is shared between the two factorizations. To control the emphasis put on the labels, a weighting factor $\lambda$ can be introduced into the objective function,

$$\|X - A_1S\|_F^2 + \lambda \|Y - A_2S\|_F^2,$$

but we focus on the cases where the approximation terms are weighted equally, $\lambda = 1$. When $\lambda = 1$, the factorization can easily be learned by performing NMF on the matrix obtained by stacking $X$ on top of $Y$, resulting in the factorization

$$[X, Y] = [A_1, A_2] S.$$

Lee et al. [12] and Haddock et al. [13] apply jNMF to semi-supervised tasks like document classification.

We apply jNMF via NMF on the matrix obtained by stacking data matrices $X_1$ and $X_2$ side-by-side, denoted by $[X_1, X_2]$, which we factorize by $[X_1, X_2] \approx A[S_1, S_2]$. This model may be represented as minimizing objective

$$\|X_1 - AS_1\|_F^2 + \|X_2 - AS_2\|_F^2$$

with respect to the factor matrices $A, S_1, S_2$. For the method to be well-defined, the data points in the two sets $X_1, X_2$ must have the same dimension.

### III. Proposed Method and Distance Measure

Our proposed distance measure identifies how well two data sets can be approximated by the common basis learned through jNMF. The existence of such a set of basis vectors indicates a similar underlying structure between the data sets. Alternatively, one may obtain a basis set in which some elements primarily contribute to the first data set and some contribute to the second, but very few are shared. This scenario suggests some structural differences in the data. In other words, there are features in one data set that are not expressed well by a basis for the other data set.

#### A. Proposed Method

Given rank $k$ jNMF approximation $[X_1, X_2] \approx A[S_1, S_2]$, our method produces a length-$k$ vector $\tilde{p}$ where each element is a measure of how often the corresponding basis vector appears in one data set or the other. These values are between -1 and 1; positive if they are used more in $X_1$ and negative if they are used more in $X_2$. For instance, a rank 3 approximation of data sets $X_1$ and $X_2$, might produce the vector $\tilde{p} = [-0.500, 0.001, 0.998]$, which indicates that the first basis vector contributes to both data sets, but appears with higher frequency in $X_2$, the second basis vector contributes equally to both data sets, and the third basis vector appears almost exclusively in $X_1$.

We compute the $i$th entry of $\tilde{p}$ with the $i$th rows of $S_1$ and $S_2$, because the magnitudes of the entries in $S_1$ and $S_2$ indicate how much this basis vector contributes to each data matrix. Our proposed method is:

1) Scale each column in $X_1, X_2$ to be mean one.

2) Learn approximation $[X_1, X_2] \approx A[S_1, S_2]$ via jNMF (1).

3) Choose threshold $T$ as

$$T \sim \text{unif} \left(\left[0, \max \left\{\max_{j}([S_1]_{1,j}), \max_{j}([S_2]_{1,j})\right\}\right]\right)$$

so that $T$ is between zero and the maximum value in the $i$th rows of $S_1, S_2$.

4) Compute $p_i := (c_{i,1,1}/n_1 - c_{i,2,1}/n_2)$, where

$$c_{i,j,k} = |\{k \mid ([S_j]_{ik}) > T\}|$$

is the number of values in the $i$th row of $S_j$ that are greater than $T$, and $n_j$ is the number of columns in $X_j$. 

5) Repeat steps 3 and 4 $K$ times and return the average vector $\tilde{p}$.

#### B. Distance Measure

Although the basis vectors and the $\tilde{p}$ vector are interpretable, a single scalar value that measures similarity or distance between two datasets is often useful. We define the distance measure between the two data matrices $X_1, X_2$ as

$$d(X_1, X_2) := \|\tilde{p}\|_1,$$

where $\tilde{p}$ is computed via the method in Subsection III-A.

We list here a few desired properties of the distance measure $d(X_1, X_2)$ and of the vector $\tilde{p}$. These properties will be experimentally verified in Subsection IV-A. Let $X_1$ be a data matrix with $n$ columns.

- **P1** Self-similarity: $d(X_1, X_1) = 0$ and $\tilde{p}$ is the zero vector.
- **P2** Permutation invariance: If $P_\pi$ is an $n \times n$ permutation matrix, $d(X_1, X_1 P_\pi) = 0$ and $\tilde{p} = 0$.
- **P3** Scaling invariance: $d(X_1, \lambda X_1) = 0$, $\tilde{p} = 0$ for $\lambda > 0$.
- **P4** Large subsets: If the columns of $X_1$ are a large subset of those of $X_1$, then $d(X_1, X_1) \approx 0$, and $d(X_1, X_1)$ decreases monotonically as the number of columns of $X_1$ approaches $n$.

$^1$To address the case where $\nu \approx 0$, we add a threshold so that $\nu \in X_i$ is only normalized if $||\nu|| \geq 0.05 \ast \text{avg}_{u \in X_i} ||u||$. 


Additive noise: If $\epsilon > 0$ is small and $N$ is a noise matrix, $d(X_1, X_1 + \epsilon N) \approx 0$ and $d(X_1, X_1 + \epsilon N)$ grows monotonically with $\epsilon$.

### IV. Empirical Results

In this section, we illustrate the proposed method and distance measure on a toy image dataset called the Swimmer dataset [14], which is composed of $11 \times 20$-pixel images such as that of Figure 1, and the 20 Newsgroups dataset [15].

Fig. 1: Sample image from the Swimmer dataset.

#### A. Distance measure properties

In this section, we verify some of the desired properties from Subsection III-B experimentally. In these experiments, we let $X_1$ be the matrix with columns that are the vectorized images from the Swimmer dataset. All Swimmer dataset experiments are run with rank $k = 10$.

We note that the distance measure $d(X_1, X_2)$ appears to exhibit the self-similarity property (P1), the permutation invariance property (P2), and the scaling invariance property (P3). As we expect, our method, when applied to $X_1$, the Swimmer data matrix, and $X_2$, identical, permuted, and scaled copies of the Swimmer data matrix, produces $\hat{p} = 0$ and $d(X_1, X_2) = 0$. See Table I.

| $X_2$ | $X_1$ | $X_1 P_{\pi}$ | $\lambda X_1$ | $X_1$ | $X_1 + N$ | $N$ |
|-------|-------|------------|-------------|-------|-----------|-----|
| $d(X_1, X_2)$ | 0.000 | 0.000 | 0.049 | 1.511 | 2.313 |

Additionally, it appears that the distance measure exhibits the large subsets property (P4) since $d(X_1, \tilde{X}_1)$ remains small when applied to the Swimmer data matrix, $X_1$, and $\tilde{X}_1$, formed as a large column subset of $X_1$. To verify this, we form $\tilde{X}_1$ as a random sample of $q\%$ of columns in $X_1$, where $q \in [88, 98]$ and plot $d(X_1, X_2)$ for each of value of $q$; see Figure 2. The distance measure also appears to exhibit the additive noise property (P5). From Figure 3, we see that the $d(X_1, X_1 + \epsilon N)$ where $N$ is a noise matrix with entries sampled i.i.d. according to distribution $\text{unif}([0, 1])$ grows monotonically with $\epsilon$. In this experiment, we plot $d(X_1, X_1 + \epsilon N)$ where $\epsilon \in [0, 1]$. The values in both experiments are averaged over fifty trials.

Fig. 2: The distance measure $d(X_1, \tilde{X}_1)$ where $X_1$ is the Swimmer data matrix and $\tilde{X}_1$ is formed as a random sample of $q\%$ of columns in $X_1$, for $q \in [88, 98]$. Values are averaged over fifty trials.

Fig. 3: The distance measure $d(X_1, X_1 + \epsilon N)$, where $X_1$ is the Swimmer data matrix, $N$ is a matrix with entries sampled i.i.d. from $\text{unif}([0, 1])$, and $\epsilon \in [0, 1]$, grows monotonically with $\epsilon$. Values are averaged over fifty trials.

We can gain some additional insight about the relationships between the data sets by looking at the basis vectors produced by the jNMF. Figure 4 shows the basis vectors and their associated $p$ scores produced by our method applied to the Swimmer data matrix $X_1$ and $X_1 + N$ where $N$ is a matrix with entries sampled i.i.d. from $\text{unif}([0, 1])$. The images with the dark background are good approximations for the basis vectors of the Swimmer data set. The basis vector in the first row on the right is used almost exclusively in the noisy data, so we may view this vector as the primary difference between
our two data sets. The method separated the basis vectors for data from noise, which was condensed into one vector.

Fig. 4: Basis vectors produced by our method applied to Swimmer data matrix $X_1$ and $X_1 + N$ where the entries in $N$ are sampled i.i.d. from \( \text{unif}([0, 1]) \). The associated $p$ values for each basis image are, reading left to right, $[0.063, -0.901, 0.076, 0.065, 0.069, 0.058, 0.058, 0.069, 0.079, 0.079]$ and $d(X_1, X_1 + N) = 1.517$ (note that this value is computed on a single trial while the corresponding entry of Table I is averaged over 50 trials). All basis vectors contribute roughly equally to both data sets, with the exception of the basis vector in the upper right, which contributes almost exclusively to the noisy data set $X_1 + N$.

### B. Swimmer experiments

Before we can use our measure to compare data sets, we must consider what it means for $d(X_1, X_2)$ to be small. Since $0 \leq |p_i| \leq 1$, the maximum value of the proposed distance measure is the rank of the jNMF approximation, $k$. We note that the distance measure is frequently significantly below this value. As a benchmark for considering the significance of these distance values, we measure the distance between our value. As a benchmark for considering the significance of that the distance measure is frequently significantly below this other distance value observed in our previous experiments, is it far below the upper bound of $k = 10$, because the random data in $N$ can be reasonably approximated with conic combinations of the structured Swimmer basis vectors. Thus, the basis vectors for the jNMF factorization of $X_1$ and $N$ do not appear too different from those in Figure 4. Despite this relatively low distance measure, $d(X_1, N)$ can serve as a baseline for interpreting $d(X_1, X_2)$ for other matrices $X_2$.

We measure the distance between the Swimmer data matrix $X_1$ and a matrix very similar in structure, the Swimmer data matrix with zeros and ones swapped, $X_2$; see Figure 5a. Note that the data points in $X_1$ can be constructed by starting with the body and adding in limbs, while those in $X_2$ can be constructed by starting with a body with all possible limbs and covering the limbs that are not being used in a particular data point. Figure 5b shows that this data set can be represented well with eight common basis vectors and two additional basis vectors, each of which is strongly associated with one data set. The common basis vectors are used differently by the two data sets; in $X_1$, they are used to add limbs to the body, while in $X_2$, they are used to cover up limbs. The method is able to identify similar structures between the two data sets as well as extracting the elements necessary to make the data sets distinct. Additionally, $d(X_1, X_2) = 2.054$, which is less than $d(X_1, N) = 2.313$, indicating that the structures of $X_1, X_2$ are similar.

### C. 20 Newsgroups experiments

As a final illustration of the promise of our proposed method and distance measure, we measure distances between the term frequency-inverse document frequency (tf-idf) representations of the various newsgroups (categories) in the 20 Newsgroups dataset [15]. The 20 Newsgroups dataset is a collection of approximately 20,000 newsgroup documents. The data set consists of six groups partitioned roughly according to subjects, with a total of 20 subgroups, and is an experimental benchmark for document classification and clustering; see e.g., [12].

In Figure 6, we visualize a heatmap with colors corresponding to average distances between samples of 100 documents of each of the twenty newsgroups, averaged over 50 trials. We remove headers, footers, and quotes from the 20 Newsgroups dataset, and then apply the tf-idf transformation to the entire set. In each trial, we sample 100 documents (represented as tf-idf vectors with length equal to the size of the entire data corpus) uniformly from each newsgroup and calculate pairwise distances between each sample. The rows and columns of the resulting distance matrix are then re-ordered and line-segregated according to cluster labels assigned by k-means with $k = 6$ applied to the columns of the distance matrix.

We note that this clustering reveals existing block structure in the distance matrix. Furthermore, we note that this clustering correctly identifies the “misc” and “comp” newsgroups. On the other hand, this clustering splits the “sci” and “rec” newsgroups into a sci.space, sci.med, rec.autos, rec.motorcycles, and sci.electronics cluster; a sci.crypt cluster; and a rec.sport.hockey and rec.sport.baseball cluster. Additionally, it combines the “alt” and “talk” newsgroups into a single cluster. While this clustering does not respect the newsgroups divisions, the clusters identified represent highly related topics.
Fig. 5: (a) Sample data points from the Swimmer data set (left) and the modified swimmer data set, where all zeros and ones are switched (right). (b) Basis vectors learned by jNMF with rank $k = 10$ on the Swimmer data set ($X_1$) with an inverted copy of the Swimmer data set such that all the zeros and ones are switched ($X_2$). Ordering the basis vectors left to right, $\bar{p} = [-0.999, 1.000, 0.010, -0.017, 0.003, -0.004, 0.015, 0.004, -0.001, -0.000]$ and $d(X_1, X_2) = 2.054$. The topmost left basis vector contributes almost exclusively to $X_2$ and the topmost right basis vector contributes almost exclusively $X_1$. The other basis vectors contribute roughly evenly to both, adding limbs to $X_1$ and removing them from $X_2$.

CONCLUSION

In this work, we have proposed a promising distance measure for datasets based on shared features learned by jNMF. Our proposed distance measure indicates similarity of two datasets and the proposed method learns which basis components are shared between the datasets and which are not. As one would hope, our proposed distance measure exhibits permutation and scaling invariance, and monotonicity over subset relationships and additive noise in the data.

Future work includes applying the measure in tasks like anomaly or plagiarism detection, as well as exploring distance measures derived from different types of matrix factorization.

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