Convex Algorithms for Nonnegative Matrix Factorization

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Abstract

We derive approximation algorithms for the nonnegative matrix factorization problem, i.e. the problem of factorizing a matrix as the product of two matrices with nonnegative coefficients. We form convex approximations of this problem which can be solved efficiently and test our algorithms on some classic numerical examples.

1 Introduction

Nonnegative matrix factorization (NMF) is a classic unsupervised technique to learn a parts-based representation of the data in an additive setting. As such, it is used as a factor analysis tool for high-dimensional data whose components are constrained to be nonnegative. Given a data matrix $A \in \mathbb{R}^{m \times n}$, we write the nonnegative matrix factorization problem as:

$$\begin{align*}
\text{minimize} & \quad \text{loss}(A, UV^T) \\
\text{subject to} & \quad U, V \geq 0,
\end{align*}$$

in the variables $U \in \mathbb{R}^{m \times k}$ and $V \in \mathbb{R}^{n \times k}$, where $\text{loss}(X, Y)$ is a loss function, and $k$ is a given rank target. This apparently simple problem can be traced back to [1] and [2] and has found many applications in machine learning and statistics. It was used for example in gene expression data analysis (see e.g. [3]), in signal processing (see [4]), as a clustering tool (see e.g. [5] and [6]), for image analysis (see [7]), etc. If $k \geq \min(m, n)$, $A = AI$ is always a solution, so our objective is to make this representation as parsimonious as possible and keep $k$ small. The decomposition is of course not unique and this and other consistency issues were explored in [7]. As a factor analysis technique, NMF is very similar to Principal Component Analysis, however PCA amounts to a simple singular value decomposition of the data matrix which is computationally easy, while NMF is a NP-Hard problem. Furthermore, in all of these applications, the nonnegativity constraint on the components is the result of some physical property of the data, hence cannot be lifted.

1.1 Current methods

Here, we briefly summarize the main types of algorithms currently used to solve it. We refer the reader to [8] for a more complete survey. The algorithms listed below have all been implemented in MATLAB libraries such as NMFLAB by [9] or NMFPACK by [10].

Multiplicative update. The original algorithm in [2], when the loss is given by the Mean Squared Error, updates the current iterates $U$ and $V$ as follows:

$$
V_{ij}^+ = V_{ij} \frac{(U^T A)_{ji}}{(U^T U V^T)_{jj}} \quad \text{and} \quad U_{ij}^+ = U_{ij} \frac{(AV)_{ij}}{(U V^T V)_{jj}}.
$$

Similar updates exist for other loss functions. This is a descent method but, in this form, it is not guaranteed to converge to a local minimum.
Gradient descent. Another set of algorithms (see [11] or [10] among others) directly apply a gradient descent algorithm to problem (1).

Alternating least squares. When the loss function is given by the MSE, a third group of algorithms take advantage of the fact that the minimization problem in only one of the variables is equivalent to a least-squares problems. These block-coordinate descent algorithms (see [12] among others) minimize the loss by alternating between the LS problems in $U$ and $V$.

Recently, [10] (see also [12]) also added a penalty term to problem (1) to make the matrices $U$ and $V$ sparse, which improves interpretability in imaging applications for example.

1.2 Contribution

All the algorithms above have one common characteristic, they all solve a nonconvex formulation of the nonnegative matrix factorization problem. In particular, this means that they all seek local solutions to the original problem. This creates stability issues, i.e. the solutions are very sensitive to the choice of initial point, it also creates complexity issues, meaning that no precise bound can be given on the computing time required to solve the problem and suboptimality cannot be measured by computing the duality gap. Here, we begin by formulating a convex approximation to nonnegative matrix factorization, we then solve the approximate problem using convex optimization methods. This means that we find global (hence potentially more stable) solutions to the approximate problem with guaranteed complexity bounds.

In the symmetric case, we first show that the NMF problem can be formulated as the problem of approximating a given matrix by a completely positive matrix. We then use a convex representation of a restriction of the set of completely positive matrices to write a convex restriction of the symmetric NMF problem. In other words, we show that solving problem (1) over a subset of all the possible choices of $U$ and $V$ is equivalent to a convex problem. We then extend these results to the nonsymmetric case.

The paper is organized as follows, in Section 2 we detail our convex approximations of problem (1) in both the symmetric and nonsymmetric case. We present some simple algorithms in Section 3. Finally, in Section 4, we compare our methods with existing algorithms in numerical examples.

2 Convex approximations

In this section we derive a convex approximation to problem (1). We first discuss the case where the matrix $A$ is symmetric, then generalize our results to nonsymmetric matrices.

2.1 Symmetric case

In this section, given a data matrix $A \in \mathbb{S}^n$, we focus on the following symmetric nonnegative matrix factorization problem:

\[
\begin{align*}
\text{minimize} & \quad \text{loss}(A, UU^T) \\
\text{subject to} & \quad U \geq 0,
\end{align*}
\]

in the variable $U \in \mathbb{R}^{n \times k}$. In this paper, we consider two classical choices for the loss function given by:

- Mean Squared Error (MSE): $\text{loss}(X, Y) = \|X - Y\|^2$
- Kullback-Leibler (KL): $\text{loss}(X, Y) = \sum_{i,j=1}^n (X_{ij} \log(X_{ij}/Y_{ij}) + Y_{ij} - X_{ij})$.

Both losses are convex functions of either $X$ or $Y$ but are not jointly convex in $(X, Y)$, which means (1) is a nonconvex problem.

2.1.1 Completely positive matrices

The solutions to this symmetric NMF problem, i.e. the symmetric matrices $A \in \mathbb{S}^n$ which can be written in the form:

\[ A = UU^T, \quad U \geq 0 \]
where $U \in \mathbb{R}^{n \times k}$, are called completely positive (see [13] for a complete discussion). This can also be written $A = \sum_{i=1}^{k} u_i u_i^T$ with $u_i \geq 0$ and the smallest $k$ for which this representation holds is called the cp-rank of $A$. This provides us with another interpretation of problem (2): it seeks the closest completely positive matrix to a given matrix $A$. It also illustrates the difficulty of this problem: the set of completely positive matrices forms a cone whose dual is the cone of copositive matrices and testing for the copositivity of a matrix is a well-known NP-Hard problem. Also, [14] shows that any continuous or binary nonconvex program can be written as a linear program over the cone of completely positive matrices. The fundamental result we use in this section is given by the following theorem.

**Theorem 1 (Th. 2.30 in [13])** If $X \in \mathbb{S}^n$ is positive semidefinite, then $\exp_H(X)$, the Hadamard (or componentwise) exponential of $X$, is completely positive.

This means that after a natural change of variables $A_{ij} = \exp(X_{ij})$, we get a sufficient, convex condition on $X$ for representation (3) to hold. This also shows that kernel matrices obtained by negative exponentiation of negative semidefinite distance matrices are completely positive, hence can be interpreted as linear kernels over nonnegative feature vectors.

### 2.1.2 Convex restriction

The above result allows us to form a convex restriction of the symmetric NMF problem in (2) as:

$$
\begin{align*}
\text{minimize} & \quad \text{loss}(A, \exp_H(X)) \\
\text{subject to} & \quad X \succeq 0,
\end{align*}
$$

in the variable $X \in \mathbb{S}^n$. When the loss function is given by the KL divergence, this problem becomes:

$$
\begin{align*}
\text{minimize} & \quad \sum_{i,j=1}^{n} A_{ij} (\log(A_{ij}) - X_{ij}) + \exp(X_{ij}) - A_{ij} \\
\text{subject to} & \quad X \succeq 0,
\end{align*}
$$

which is a convex optimization problem in the variable $X \in \mathbb{S}^n$. When the loss is given by the MSE, the objective function is not convex in $X$ unless we impose the additional constraint that $A_{ij}/2 \leq \exp(X_{ij})$. Problem (4) then becomes:

$$
\begin{align*}
\text{minimize} & \quad \sum_{i,j=1}^{n} (\exp(X_{ij}) - A_{ij})^2 \\
\text{subject to} & \quad A_{ij}/2 \leq \exp(X_{ij}), \quad i, j = 1, \ldots, n
\end{align*}
$$

which is also a convex problem in the variable $X \in \mathbb{S}^n$.

### 2.1.3 Factorizing $\exp_H(X)$ when $X$ is positive semidefinite

We know from Theorem 1 that $\exp_H(X)$ is completely positive when $X$ is positive semidefinite so there is a matrix $L$ such that

$$
\exp_H(X) = UU^T,
$$

where $U \in \mathbb{R}^{n \times k}$. First, Carathéodory’s theorem allows us to bound the size of $U$ (i.e. the cp-rank of $\exp_H(X)$), and Theorem 3.5 in [13] shows that we can get:

$$
\begin{align*}
k & \leq \frac{r^2 + 1}{2} - 1,
\end{align*}
$$

where $r = \text{Rank}(\exp_H(X))$. Also, the Hadamard (or componentwise) product of two completely positive matrices is completely positive: suppose $A = \sum_{i=1}^{k} a_i a_i^T$ and $B = \sum_{i=1}^{l} b_i b_i^T$ with $a_i, b_i \geq 0$, then:

$$
A \circ B = \sum_{i=1}^{k} \sum_{j=1}^{l} (a_i \circ b_j)(a_i \circ b_j)^T,
$$

hence the Hadamard product $A \circ B$ is completely positive as the sum of nonnegative rank one matrices. Now, because $X$ is positive semidefinite, we can write:

$$
\exp_H(X) = \prod_{i=1}^{n} \exp_H \left( \lambda_i x_i x_i^T \right),
$$

where $\lambda_i$ are the eigenvalues of $X$.
where the matrix product is understood componentwise and \( \lambda_i \in \mathbb{R}_+^n \), which means that \( \exp_H(X) \) can be written as the Hadamard product of matrices of the type \( \exp_H(vv^T) \). As in [13] Theorem 2.30, we let \( M = \max_{i=1,\ldots,n} |v_i| \), then

\[
\exp_H(vv^T)_{ij} = \exp(v_i v_j) = \exp(-M^2 + (M + x_i)(M + x_j) - M(x_i + x_j)),
\]

so

\[
\exp_H(vv^T) = \exp(-M^2) \exp_H(yy^T) \circ zz^T,
\]

where \( y = M1 + v \) and \( z = \exp(-Mv) \) are both nonnegative vectors. Because \( y \) is nonnegative and

\[
\exp_H(yy^T) = \sum_{i=1}^{\infty} \frac{(yy^T)^{oi}}{i!},
\]

with \( (yy^T)_{ij} = (y_i y_j)^k \), the matrix \( \exp_H(yy^T) \) is completely positive. Hence, as the Hadamard product of two completely positive matrices, \( \exp_H(vv^T) \) is completely positive. To summarize, when \( X \) is positive semidefinite, we factorize the matrix \( \exp_H(X) \) as follows:

**Factorizing \( \exp_H(X) \)**

1. Compute the eigenvalue decomposition: \( X = \sum_{i=1}^{n} \lambda_i x_i x_i^T \).
2. Decompose each factor, \( \exp_H(v_i v_i^T) = \exp(-M^2) \exp_H(y_i y_i^T) \circ z_i z_i^T \) where \( v_i = \sqrt{\lambda_i} x_i \) and \( y_i, z_i \) are nonnegative vectors.
3. Approximate \( \exp_H(y_i y_i^T) \) as \( \sum_{k=1}^{k} (yy^T)^{2k} / k! \).
4. Collect all the terms above using the chain rule in (8) to get \( \exp_H(X) = UU^T \).

Without any further processing, the size of \( U \) can quickly become very large. Because of the bound given in (7), we know however that the number of columns of \( U \) is bounded above by \( r(r + 1)/2 - 1 \) where \( r = \text{Rank}(\exp_H(X)) \) and we can use this result to simplify the decomposition, but this is numerically costly and typically unnecessary. In practice, the eigenvalues of \( \exp_H(v_i v_i^T) \) are decreasing exponentially fast and we can use the fact that when \( X \in \mathbb{S}^n \) is a positive semidefinite matrix with nonnegative coefficients and \( \text{Rank}(X) = 2 \), then \( X \) is completely positive. We then replace \( \exp_H(v_i v_i^T) \) by a rank two approximation which, if it is nonnegative, means that the size \( k \) of the matrix \( U \in \mathbb{R}^{n \times k} \) is given by \( k = 2^r \) where \( r \) is the number of significant factors in \( X \), which is typically small. The precision of that approximation is further studied in Section 4.

### 2.2 Sparse decomposition

As suggested in [10] (see also [12]), e.g. when the matrix \( A \) itself is sparse, we look for a **sparse** decomposition \( A = UU^T \), i.e. a decomposition where the matrices \( U \) are sparse. In that case, the change of variable \( A = \exp(X) \) is not appropriate. We can however look directly for a low rank decomposition by exploiting the property detailed above that when \( X \in \mathbb{S}^n \) is a positive semidefinite matrix with nonnegative coefficients and \( \text{Rank}(X) = 2 \), then \( X \) is completely positive. We then solve:

\[
\begin{align*}
\text{minimize} & \quad ||A - X||^2 + \gamma |X| + \nu \text{Tr}(X) \\
\text{subject to} & \quad X \succeq 0, \ X \succeq 0,
\end{align*}
\]

in the variable \( X \in \mathbb{S}^n \), where \( |X| = \sum_{i,j=1}^{n} |X_{ij}| \), \( \gamma \) is a parameter controlling the sparsity of \( X \) and \( \nu \) is a penalty on its rank (see [15] for details).

### 2.3 Recursive decomposition

Because the condition in Theorem [1] is only sufficient, problems (5) and (6) only cover a subset of all the possible nonnegative factorizations of the data matrix \( A \). To overcome this limitation, we can solve problem (2) recursively, setting \( A_0 = A \) and

\[
A_{k+1} = A_k - U_k U_k^T
\]

where \( U_k \) is the solution to the factorization problem given \( A_k \). To ensure, that the intermediate matrices \( A_k \) remain nonnegative, we can simply add the (convex) constraint that \( U_k U_k^T \leq A \) to problems (5) and (6).
We now extend the results of the previous section to the symmetric case. Given a data matrix $A \in \mathbb{R}^{m \times n}$, we write the nonnegative matrix factorization problem as:

$$\begin{align*}
\text{minimize} & \quad \text{loss}(A, UV^T) \\
\text{subject to} & \quad U, V \geq 0,
\end{align*}$$

in the variables $U \in \mathbb{R}^{m \times k}$ and $V \in \mathbb{R}^{n \times k}$, where $\text{loss}(X, Y)$ is one of the loss functions given above. Because the matrix $A$ has a nonnegative factorization if and only if there are matrices $B, C \in \mathbb{S}^n$ such that the symmetric block-matrix:

$$\begin{pmatrix} B & A \\ A^T & C \end{pmatrix}$$

is completely positive. Of course any nonnegative matrix can be factorized as the product of two nonnegative matrices because $A = AI$ is always a solution. Our objective here is to make this representation as parsimonious as possible and find a solution with minimum cp-rank. We can’t minimize the cp-rank of the decomposition directly without making the problem nonconvex, however the bound in (7) shows that we can use the rank of a matrix as a proxy for its cp-rank. We know from [15] that when $X \in \mathbb{R}^{m \times n}$, $\|X\|_*$, the trace norm of $X$ is the largest convex lower bound on $\text{Rank}(X)$. We also know that $\|X\|_* \leq t$ if and only if there are symmetric matrices $Y, Z$ such that:

$$\begin{pmatrix} Y & X \\ X^T & Z \end{pmatrix} \succeq 0 \quad \text{and} \quad \text{Tr}(Y) + \text{Tr}(Z) \leq 2t.$$

The problem of finding a low cp-rank nonnegative factorization of a matrix $A \in \mathbb{R}^{m \times n}$ can then be written:

$$\begin{align*}
\text{minimize} & \quad \text{loss}(A, X) + \gamma(\text{Tr}(Y) + \text{Tr}(Z)) \\
\text{subject to} & \quad \begin{pmatrix} Y & X \\ X^T & Z \end{pmatrix} \text{ completely positive},
\end{align*}$$

in the variables $X \in \mathbb{R}^{m \times n}$, $Y \in \mathbb{S}^m$ and $Z \in \mathbb{S}^n$, where $\gamma \geq 0$ controls the rank of the solution. This is now a symmetric NMF problem and can be solved using the results detailed in the previous sections.

### 3 Algorithms

The results in (5) and (6) show that the symmetric NMF problem can be approximated by convex problems for which efficient, globally convergent algorithms are available. Here, because our focus is on solving large-scale problems with a relatively low precision, we use simple first-order methods to solve the optimization problems detailed in Section 2.

#### 3.1 Projected gradient method

The simplest of these algorithms is the projected gradient method. Suppose that we need to minimize a convex function $f(x)$ over a convex set $C$. The projected gradient algorithms works as follows:

**Projected Gradient Method**

1. Start from a point $x_0 \in \mathbb{R}^n$.
2. Compute $x_{k+1} = p_C(x_k + \nabla f(x_k))$, where $p_C(x)$ is the projection of $x$ on the set $C$.
3. Repeat step 2 until precision target is reached.

Applying this method to problem (5) for example, to solve:

$$\begin{align*}
\text{minimize} & \quad \sum_{i,j=1}^n A_{ij} (\log(A_{ij}) - X_{ij}) + \exp(X_{ij}) - A_{ij} \\
\text{subject to} & \quad X \succeq 0,
\end{align*}$$

we get $p_C$ explicitly as $p_C(X) = X_+$, where the matrix $X_+$ is obtained by zeroing out the negative eigenvalues of the matrix $X$. 

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5
3.2 Complexity

Provided some smoothness assumptions on the objective function, the number of iterations of the generic projected gradient method grows as $O(1/\epsilon^2)$ where $\epsilon$ is the target precision.

3.3 Convergence and duality gap

The dual of problem (5) is given by:

$$\text{maximize} \quad \sum_{i,j=1}^{n} A_{ij} + Y_{ij} - (A_{ij} + Y_{ij}) \log(A_{ij} + Y_{ij})$$

subject to

$Y \succeq 0$, \quad (12)

in the variable $Y \in S^n$. The optimality conditions impose:

$$Y = \exp_H(X) - A \succeq 0,$$

where $X,Y$ are primal and dual solutions to (5). This means that if $X$ is the current primal point, then $(\exp_H(X) - A)_+$ is a dual feasible point which can be used to compute a duality gap, measure the optimality of $X$ and track convergence.

4 Numerical Results

In this section, we test the performance of our algorithm for solving the symmetric NMF problem on graph partitioning problems.

4.1 Graph partitioning using NMF

Let $A \in \{0, 1\}^{n \times n}$ be the adjacency matrix of a given graph $G$, with

$$A_{ij} = \begin{cases} 1 & \text{if } (i, j) \text{ is an edge of } G \\ 0 & \text{otherwise.} \end{cases}$$

Suppose that we want to partition this graph into $k$ clusters $C_k$ while minimizing the number of graph edges between clusters and maximizing the number of graph edges inside clusters. For a given partition $C$ of a graph with adjacency matrix $A \in \{0, 1\}^{n \times n}$, the performance measure we use here is given by:

$$\text{perf}(C) = 1 - \frac{\# \left\{ (i, j) \mid A_{ij} \neq \sum_{l=1}^{k} X_{il}X_{jl} \right\}}{n^2}$$

(13)

where $X \in \{0, 1\}^{n \times k}$ is an indicator matrix such that:

$$X_{ik} = \begin{cases} 1 & \text{if node } i \text{ is in cluster } C_k \\ 0 & \text{otherwise,} \end{cases}$$

which satisfies $X1 = 1$. The graph partitioning problem can then be formulated as:

$$\text{minimize} \quad \|A - XX^T\|^2$$

subject to \quad $X1 = 1$, \quad (14)

in the variables $X \in \{0, 1\}^{n \times k}$. This is a (hard) binary optimization problem, which we relax into a symmetric nonnegative matrix factorization problem as in [16], to get:

$$\text{minimize} \quad \|A - XX^T\|^2$$

subject to \quad $X \geq 0$, \quad (15)

in the variable $X \in \mathbb{R}^{n \times k}$, which can be solved using the algorithms detailed in Section [3]. We can then turn the solution $X$ of this relaxation into an indicator matrix by setting the maximum coefficient of each row to one and all the others to zero.
4.2 Partitioning performance

To test the performance of our algorithms for symmetric NMF on graph partitioning problems, we generate random graphs whose adjacency matrices have given block sparsity patterns. We generate three uniform random matrices \( A, B \in \mathbb{S}^n \) and \( C \in \mathbb{R}^{n \times n} \) and use two parameters \( \alpha, \beta \in [0, 1] \) to control the sparsity and form a sample graph adjacency matrix as:

\[
\begin{pmatrix}
1\{A_{ij} \geq \alpha\} & 1\{C_{ij} \geq \beta\} \\
1\{C_{ij} \geq \beta\} & 1\{B_{ij} \geq \alpha\}
\end{pmatrix}
\]

then randomly permute the matrix. An example is detailed in Figure 1. We then compare the performance of our code with that of spectral clustering (see [17] for example) and show the results in Figure 2 below. We observe that both methods perform similarly well on clearly clustered data but that the NMF solution dominates spectral clustering as the graphs become closer to bipartite.

4.3 Convergence speed

In Figure 2 we plot number of iterations of the projected gradient algorithm versus matrix size \( n \) in randomly generated problems for various problem sizes.

![Figure 1: Graph partitioning example: original (randomly generated) adjacency matrix on the left, clustered permutation on the right obtained by solving problem (15) using the algorithms in Section 3](image)

![Figure 2: Left: Average number of iterations versus matrix size for the projected gradient algorithm. Right: Average performance versus graph connectivity for spectral clustering (squares) and the solution to the NMF problem (15) using the algorithms in Section 3 (circles, dashed lines at plus and minus one standard deviation).](image)
4.4 Extensions

While the results in the symmetric case seem to perform very well in numerical experiments, this is not the case for nonsymmetric problems where alternating projection methods using highly optimized interior point solvers are still at least an order of magnitude faster than our method. At this point, efficiently exploiting the NMF representation detailed here in the nonsymmetric case remains an open numerical problem.

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