Fast and Effective Algorithms for Symmetric Nonnegative Matrix Factorization

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Abstract

Symmetric Nonnegative Matrix Factorization (SNMF) models arise naturally as simple reformulations of many standard clustering algorithms including the popular spectral clustering method. Recent work has demonstrated that an elementary instance of SNMF provides superior clustering quality compared to many classic clustering algorithms on a variety of synthetic and real world data sets. In this work, we present novel reformulations of this instance of SNMF based on the notion of variable splitting and produce two fast and effective algorithms for its optimization using i) the provably convergent Accelerated Proximal Gradient (APG) procedure and ii) a heuristic version of the Alternating Direction Method of Multipliers (ADMM) framework. Our two algorithms present an interesting tradeoff between computational speed and mathematical convergence guarantee: while the former method is provably convergent it is considerably slower than the latter approach, for which we also provide significant but less stringent mathematical proof regarding its convergence. Through extensive experiments we show not only that the efficacy of these approaches is equal to that of the state of the art SNMF algorithm, but also that the latter of our algorithms is extremely fast being one to two orders of magnitude faster in terms of total computation time than the state of the art approach, outperforming even spectral clustering in terms of computation time on large data sets.

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1 Introduction

In graph-based clustering approaches, data points are treated as individual nodes in a graph whose edges are weighted using some similarity function. These weights are stored in a symmetric $n \times n$ adjacency matrix $A$ whose $(i, j)^{th}$ entry $A_{ij}$ denotes the similarity between the $i^{th}$ and $j^{th}$ data points (or nodes)$^{1}$. A common approach for separating the graph into $K$ clusters is via an approximate factorization $A \approx LL^T$, where $L$ is an $n \times K$ nonnegative matrix. The $i^{th}$ data point is then assigned to the $k^{th}$ cluster where $k$ is the index of the largest entry of the $i^{th}$ row of $L$. This factorization is obtained through solving the Symmetric Nonnegative Matrix Factorization (SNMF) problem defined as

$$\min_{L} \|A - LL^T\|_F^2$$
subject to $L \geq 0$, \hspace{1cm} (1)

where $\|\cdot\|_F$ denotes the Frobenius norm and the nonnegativity constraint is taken element-wise. SNMF has been shown to have superior clustering efficacy compared to a number of data-clustering and graph-clustering algorithms (Kuang et al, 2012; He et al, 2011; Yang et al, 2012; Yang and Oja, 2012, 2011). Moreover, slight variations of the SNMF formulation in (1) have been shown to be equivalent to a variety of clustering algorithms including K-means, Nonnegative Matrix Factorization, as well as several normalized spectral clustering approaches (von Luxburg, 2007; Ding et al, 2005, 2008). Due to its efficacy and its myriad of connections to other powerful clustering approaches, efficient algorithms for solving the SNMF model in (1) are of particular value to the practicing data-miner. However, while an array of algorithms have been developed for the parent problem of Nonnegative Matrix Factorization (NMF) and NMF-related problems (Berry et al, 2007; Hoyer, 2004; Lin, 2007; Seung and Lee, 2001; Zhang, 2010; Xu et al, 2012), few specialized algorithms have so far been developed for solving (1). This is due to the fact that the SNMF problem, while having fewer variables to solve for than the standard NMF formulation, is more challenging to solve due to the forced equality between the two matrix factors.

$^{1}$One common example of a similarity function is the Gaussian similarity which gives the $(i, j)^{th}$ entry of $A$ as $A_{ij} = \exp\left(-\|d_i - d_j\|_2^2/2\sigma^2\right)$ where $d_i$ and $d_j$ are the $i^{th}$ and $j^{th}$ data points, respectively, and $\sigma > 0$ is a tuning parameter that is typically set in proportion to the distribution of the given data.
In this paper we develop two novel algorithms for SNMF based on the notion of variable splitting combined with classic approaches to constrained numerical optimization, namely, the Quadratic Penalty Method (QPM) \cite{nocedal2006numerical} with solution via the provably convergent Accelerated Proximal Gradient (APG) method \cite{beck2009fast,parikh2013proximal}, and a heuristic form of the Alternating Direction Method of Multipliers (ADMM) framework \cite{boyd2011distributed}. Not only do our algorithms typically outperform the current state of the art method developed in \cite{kuang2012spectral} in terms of clustering efficacy, but the latter algorithm additionally runs on average one to two orders of magnitude faster in terms of computation time on medium-sized data sets consisting of several thousand data points, and can even outperform spectral clustering in terms of run time on larger data sets.

The remainder of this paper is organized as follows: in the next section we briefly review popular data- and graph-based clustering approaches as well as the current state of the art algorithm for solving the standard SNMF model in (1). In section 3 we introduce and derive our two proposed algorithms based on the notion of variable splitting. We then discuss the computation time complexity of our fast ADMM based algorithm and compare it to the state of the art Newton-like procedure in section 4. The fifth section contains experiments on synthetic and real data which illustrate the efficacy and extreme efficiency of our proposed approaches. We then conclude with brief reflections in section 6. The appendix of this work then contains critical mathematical details regarding our first approach, as well as strong mathematical proof regarding the convergence of our second algorithm.

2 Review of matrix factorization-based clustering approaches

In this section we review state of the art data and graph-based clustering approaches. In addition we highlight many important connections that exist between this wide array of techniques, which illustrates how the SNMF problem of interest in this work relates to other methods via the framework of matrix factorization.
2.1 Spectral clustering

Spectral clustering is an immensely popular graph-based clustering approach that groups \( n \) given data points via spectral analysis of the graph Laplacian matrix \( U \) associated to an input \( n \times n \) adjacency matrix \( A \). This Laplacian is given by

\[
U = D - A,
\]

where \( D \) is the diagonal degree matrix with the \( i^{th} \) diagonal entry given by \( D_{ii} = \sum_{j=1}^{n} A_{ij} \), where \( A_{ij} \) denotes the \((i, j)^{th}\) entry of \( A \). The Laplacian matrix \( U \) is symmetric positive semi-definite, and hence can be diagonalized by an orthogonal basis of eigenvectors, the top \( K \) of which stacked column-wise form a closed form solution to the unconstrained symmetric matrix factorization problem

\[
\min_{L} \|U - L L^T\|_F^2.
\]

In the spectral clustering framework data is partitioned into \( K \) clusters via the \( K \) eigenvectors of \( U \) (corresponding to its smallest \( K \) eigenvalues), which are stacked column-wise into a matrix. The final clustering assignments are then made by performing K-means on the rows of this matrix (von Luxburg, 2007).

A popular normalized version of spectral clustering replaces \( U \) with a normalized version given by

\[
U \leftarrow D^{-1/2} U D^{-1/2},
\]

where \( D^{-1/2} \) denotes the diagonal matrix whose entries are the square root of the corresponding entries of the inverse of \( D \), and then follows the same strategy for assigning the data points to their respective clusters. This simple adjustment to spectral clustering works significantly better in practice (Ng et al, 2002). Additionally, as mentioned in the introduction section, this normalized version has very close connections to kernelized K-means and SNMF (see e.g., Theorem 5 of (Ding et al, 2005)).

2.2 Nonnegative Matrix Factorization (NMF)

NMF has been shown to be an effective approach for both dimension reduction and data-based clustering applications. Formally, in both applications
of NMF, we look to recover the factorized approximation to an \( n \times m \) data matrix \( H \) of the form \( XY^T \) by solving the standard recovery problem below

\[
\begin{align*}
\min_{X,Y} & \quad \|H - XY^T\|_F^2 \\
\text{subject to} & \quad X, Y \geq 0,
\end{align*}
\]

where \( X \) is an \( n \times K \) matrix, \( Y \) is an \( m \times K \) matrix and both are constrained to be nonnegative. When employed in clustering applications the matrix \( H \) typically contains the raw data itself (Arora et al., 2011; Berry et al., 2007) and the hypothesized number of clusters \( K \) into which the data lies is set as the number of columns for both matrices \( X \) and \( Y \). The \( i^{th} \) data point is then assigned to the \( k^{th} \) cluster where \( k \) is the index of the largest entry of the \( i^{th} \) row of the recovered \( Y \) matrix. NMF is directly related to the problem of Dictionary Learning, popular in the signal processing and machine learning communities (see e.g., (Aharon et al., 2005) and references therein) where a factorization is desired with the coefficient matrix \( Y \) is constrained to be sparse. Furthermore both the NMF and Dictionary Learning problems can be thought of as variations of the basic K-means paradigm, where each column of \( X \) corresponds to an individual centroid location and each row of \( Y \) is a point’s centroid assignment (Aharon et al., 2006; Ding et al., 2010).

### 2.3 Symmetric Nonnegative Matrix Factorization (SNMF)

The elementary SNMF problem in (1), where the matrix \( A \) is an \( n \times n \) adjacency matrix, has been shown to be very effective in graph-based clustering applications. Using an array of synthetic and real data sets several works (Kuang et al., 2012; He et al., 2011; Yang et al., 2012; Yang and Oja, 2012, 2011) have shown that algorithms which can solve the SNMF problem produce superior clustering quality compared with standard algorithms including: normalized spectral clustering as discussed in section 2.1, K-means, as well as NMF (see section 2.2).

One popular and highly efficient algorithm used by (Kuang et al., 2012) for solving the SNMF problem is a simple projected Newton-like method which the authors refer to as SymNMF. Denoting by \( f(L) = \|A - LL^T\|_F^2 \) the objective function of the SNMF problem and \( S \) is an approximation to the Hessian \( \nabla^2 f(L) \), SymNMF takes projected descent steps of the form
\[ x^k = [x^{k-1} - \alpha_k S \nabla f(x^{k-1})]^+ \] \tag{6}

where \( \alpha_k \) is a steplength tuned at each iteration by a standard adaptive procedure (see e.g., (Luenberger and Ye, 2008)) to ensure descent at each step, and the positive part operator \([\cdot]^+\) sets all negative entries of its input to zero. As is always the case with Newton approximation schemes, the finer \( S \) approximates the true Hessian of \( f \) (i.e., as \( S \approx \nabla^2 f(L) \) becomes more accurate) the more rapid is the convergence of the scheme (Wright and Nocedal, 1999), but the higher the memory and computation overhead of each step. In their work (Kuang et al, 2012) the authors offer several Hessian approximations schemes that aim at rapid convergence with minimal overhead.

3 Proposed methods

In this section we propose two approaches to solving the SNMF problem in (1) based on the notion of variable splitting, an extremely popular reformulation technique in signal and image processing (see e.g., (Goldstein and Osher, 2009; Afonso et al, 2010; Boyd et al, 2011)). In the first instance we propose to solve a quadratic-penalized relaxation of the original problem, whereas in the second approach we aim at solving the original problem itself.

3.1 Variable splitting and relaxation

Taking the original model in equation (1) we split the variable \( L \) by introducing a surrogate variable \( Z \), giving the equivalent problem

\[
\begin{align*}
\text{minimize} & \quad \| A - LZ^T \|_F^2 \\
\text{subject to} & \quad L, Z \geq 0 \\
& \quad L - Z = 0.
\end{align*}
\] \tag{7}

Note that we have explicitly constrained \( Z \geq 0 \), even though this constraint seems redundant since \( L \) is already constrained to be nonnegative and \( Z \) is constrained to be equal to \( L \). However it will not be redundant when we relax the problem by squaring the equality constraint and bringing it to the objective as

\[
\begin{align*}
\text{minimize} & \quad \| A - LZ^T \|_F^2 + \rho \| L - Z \|_F^2 \\
\text{subject to} & \quad L, Z \geq 0.
\end{align*}
\] \tag{8}
This approach to approximating a constrained optimization problem, known as the Quadratic Penalty Method (QPM), is widely used in numerical optimization. In particular, as $\rho \rightarrow \infty$ one can show formally that solving this problem is equivalent to solving the constrained problem in (7), and hence the original SNMF problem itself shown in (1). Generally speaking, however, it is common to set $\rho$ to only a moderate value in practice as this typically provides a solution to the QPM form of a problem that solves the original problem very well for many applications (Nocedal and Wright, 2006). In our experiments we have found this to be the case for the SNMF problem as well (see Section 5). Finally, note how this relaxed form of the SNMF problem can also be thought of as a regularized form of the standard NMF problem in (5), and is precisely this problem when $\rho = 0$.

3.2 Accelerated Proximal Gradient (APG) approach

We solve (8) by alternatingly minimizing over $L$ and $Z$, in each case to convergence, which in turn produces a provably convergent approach (Berry et al., 2007). In order to do this we employ (in each direction) the Accelerated Proximal Gradient (APG) method (Beck and Teboulle, 2009; Parikh and Boyd, 2013). In the $L$ direction the standard proximal gradient step, a descent step projected onto the nonnegative orthant, takes the form

$$L^{i+1} = \left[ L^i - \alpha \left( \left( L^i (Z)^T - A \right) Z + \rho (L^i - Z) \right) \right]^+, \quad (9)$$

where the steplength $\alpha$ can be optimally set (see section 7.1) as the reciprocal of the Lipschitz constant of the objective in (8) in $L$ as

$$\alpha = \frac{1}{\| (Z)^T Z + \rho I \|_2}. \quad (10)$$

The update procedure in (9) is repeated until convergence. Collecting all terms in $L^i$, (9) can be written in a more computationally efficient manner as

$$L^{i+1} = \left[ L^i \left( (1 - \alpha \rho) I - \alpha (Z)^T Z \right) + \alpha (A + \rho I) Z \right]^+, \quad (11)$$

since the matrices $(1 - \alpha \rho) I - \alpha (Z)^T Z$ and $\alpha (A + \rho I) Z$ may be cached and reused at each iteration. Written in this way, the accelerated form of the proximal gradient step (which is provably an order faster in terms of
convergence\textsuperscript{2}) can be written as

\[
L^{i+1} = \left[ \Phi^i \left( (1 - \alpha \rho) I - \alpha (Z^T Z) + (A + \rho I) Z \right) \right]^+
\]
\[
\Phi^{i+1} = L^{i+1} + \frac{i}{i+3} (L^{i+1} - L^i).
\]  

Using precisely the same ideas, we may write the accelerated proximal gradient step in \( Z \) as

\[
Z^{j+1} = \left[ \Psi^j \left( (1 - \beta \rho) I - \beta (L^T L) + (A^T + \rho I) L \right) \right]^+
\]
\[
\Psi^{j+1} = Z^{j+1} + \frac{j}{j+3} (Z^{j+1} - Z^j),
\]  

where again the steplength \( \beta \) may be optimally set (see section 7.1) as the reciprocal of the Lipschitz constant of \( (8) \) in \( Z \) as

\[
\beta = \frac{1}{\| (L)^T L + \rho I \|^2_F}.
\]  

For convenience we reproduce the entire alternating accelerated proximal gradient approach we employ in Algorithm 1, which we refer to as \text{SNMF}_{\text{APG}}.

### 3.3 Alternating Direction Method of Multipliers approach

We reformulate problem \( (1) \) slightly differently than in the previous instance, splitting the variable \( L \) twice as

\[
\min_{L,X,Y} \frac{1}{2} \| A - XY^T \|^2_F
\]

subject to \( L \geq 0 \)

\[
L - X = 0
\]

\[
L - Y = 0.
\]  

This is again an equivalent reformulation of the original problem in equation \( (1) \). However unlike the use of APG method previously taken where we

\textsuperscript{2}Standard proximal gradient descent is provably convergent to within \( \frac{1}{k} \) of a minimum in \( O(k) \) iterations, while APG is convergent to within \( \frac{1}{k^2} \) in the same order of steps (Beck and Teboulle, 2009; Watt et al, 2016).
Algorithm 1 SNMF\textsubscript{APG}

\textbf{Input:} Adjacency matrix $A$, penalty parameter $\rho > 0$, stopping threshold $\epsilon$, and initializations for $Z^0$, $\Phi^0$, and $\Psi^0$

\textbf{Output:} Final point-assignment matrix $Z^k$

$k \leftarrow 1$

While $\frac{\|L^k - L^{k-1}\|_F}{\|L^{k-1}\|_F} + \frac{\|Z^k - Z^{k-1}\|_F}{\|Z^{k-1}\|_F} > \epsilon$:

\hspace{1em} (update $L$)

Compute the Lipschitz constant $\alpha_k = \frac{1}{\| (Z^{k-1})^T Z^{k-1} \|_2}$

Reset the counter for the following while loop $i \leftarrow 0$

While $\frac{\|L^i - L^{i-1}\|_F}{\|L^{i-1}\|_F} > \epsilon$:

\hspace{2em} $R^{i+1} = \Phi^i \left( (1 - \alpha_{k-1} \rho) I - \alpha_{k-1} (Z^{k-1})^T Z^{k-1} \right) + \alpha_{k-1} (A + \rho I) Z^{k-1}$

\hspace{2em} $L^{i+1} = [R^{i+1}]^+$

\hspace{2em} $\Phi^{i+1} = L^{i+1} + \frac{i}{i+3} (L^{i+1} - L^i)$

End

$L^k \leftarrow L^{i+1}$

\hspace{1em} (update $Z$)

Compute the Lipschitz constant $\beta_k = \frac{1}{\| (L^k)^T L^k + \rho I \|_2}$

Reset the counter for the following while loop $j \leftarrow 0$

While $\frac{\|Z^j - Z^{j-1}\|_F}{\|Z^{j-1}\|_F} > \epsilon$:

\hspace{2em} $S^{j+1} = \Psi^j \left( (1 - \beta_k \rho) I - \beta_k (L^k)^T L^k \right) + \beta (A^T + \rho I) L^k$

\hspace{2em} $Z^{j+1} = [S^{j+1}]^+$

\hspace{2em} $\Psi^{j+1} = Z^{j+1} + \frac{j}{j+3} (Z^{j+1} - Z^j)$

End

$Z^k \leftarrow Z^{j+1}$

$k \leftarrow k + 1$

End

aimed to solve a relaxed form of the SNMF problem, here we aim to solve this reformulated version of the exact problem itself via a primal-dual method known as the Alternating Direction Method of Multipliers (ADMM).
While developed close to a half a century ago, ADMM and other Lagrange multiplier methods in general have seen an explosion of recent interest in the machine learning and signal processing communities (Boyd et al., 2011; Goldstein and Osher, 2009). While classically ADMM has been provably convergent for only convex problems, recent work has also proven convergence of the method for particular families of nonconvex problems (see e.g., (Zhang, 2010; Xu et al., 2012; Hong et al., 2014; Magnusson et al., 2014)). There has also been extensive successful use of ADMM as a heuristic method for highly nonconvex problems (Xu et al., 2012; Zhang, 2010; Watt et al., 2014; Boyd et al, 2011; Barman et al, 2011; Derbinsky et al, 2013; Fu and Banerjee, 2013; You and Peng, 2014). It is in this spirit that we have applied ADMM to our nonconvex problem and, like these works, find it to provide excellent results empirically (see section 5). Furthermore, the specific reformulation we have chosen in (15) where we have used two splitting variables X and Y, allows us to prove a significant result regarding convergence of ADMM applied to this reformulation, i.e., any fixed point of our algorithm is indeed a KKT point of the original problem (see the Appendix for a proof). This type of result has in fact been shown to hold when applying ADMM to other matrix factorization problems as well (see e.g., (Xu et al., 2012; Zhang, 2010)).

Forming the Augmented Lagrangian associated to (15) gives

\[ L(X, Y, L, \Lambda, \Gamma, \rho) = \frac{1}{2} \| A - XY^T \|_F^2 + \frac{\rho}{2} \| L - X \|_F^2 + \Lambda \cdot (L - X) + \frac{\rho}{2} \| L - Y \|_F^2 + \Gamma \cdot (L - Y), \]

(16)

where \( \langle \cdot, \cdot \rangle \) denotes the inner-product of its input matrices and \( \rho > 0 \) is a parameter that typically requires only a small amount of tuning in practice (see Section 5 for further discussion). We will alternate minimizing \( L \) over primal variables \( X, Y, \) and \( L \) with a gradient ascent step in the dual variables \( \Lambda \) and \( \Gamma \). Over \( X \) this reduces to the simple constrained minimization (after combining terms in \( X \) and ignoring all others) of the form

\[ \min_X \frac{1}{2} \| XY^T - A \|_F^2 + \frac{\rho}{2} \| X - \left( L + \frac{1}{\rho} \Lambda \right) \|_F^2, \]

(17)

which is a simple unconstrained quadratic problem. Setting its gradient to zero gives the optimal solution as

\[ X^* = (AY + \rho L + \Lambda) \left( Y^T Y + \rho I \right)^{-1}. \]

(18)

The invertibility of the rightmost matrix above is assured due to the addition of the weighted identity \( \rho I \) to \( Y^T Y \). Similarly, minimizing the Lagrangian
in (16) over $Y$ reduces to solving another simple quadratic problem given below

$$
\min_Y \frac{1}{2} \|XY^T - A\|_F^2 + \frac{\rho}{2} \|Y - \left( L + \frac{1}{\rho} \Gamma \right) \|_F^2.
$$

(19)

Again, setting the gradient to zero gives the optimal solution

$$
Y^* = \left( AX + \rho L + \Gamma \right) \left( X^TX + \rho I \right)^{-1}.
$$

(20)

Note that in practice rarely do we solve for $Y^*$ by actually inverting the matrix $X^TX + \rho I$ as in (20). Instead, it is more efficient to catch a Cholesky factorization of this matrix and solve the corresponding linear system using forward-backward substitution.

Finally, over $L$ we have the quadratic minimization problem with a non-negativity constraint

$$
\min_L \left\| L - \left( X - \frac{1}{\rho} \Lambda \right) \right\|_F^2 + \left\| L - \left( Y - \frac{1}{\rho} \Gamma \right) \right\|_F^2
$$

subject to $L \geq 0$.

(21)

Completing the square in $L$ above, the problem becomes a projection onto the positive orthant defined by $L \geq 0$, whose solution is simply given by

$$
L^* = \frac{1}{2} \left[ X - \frac{1}{\rho} \Lambda + Y - \frac{1}{\rho} \Gamma \right]^+.
$$

(22)

Together with the dual ascent steps we have the full ADMM algorithm as summarized in Algorithm 2, which from now on is referred to as the SNMF$_{ADMM}$ algorithm.

4 Time complexity analysis

In this section we compute the per iteration complexity of SNMF$_{ADMM}$ - the fastest of our two proposed algorithms - and compare it to the per iteration cost of the state of the art SNMF approach mentioned in section 2.3. As can be seen in Algorithm 2, each iteration of SNMF$_{ADMM}$ includes updating primal variables $X$, $Y$, and $L$, and dual variables $\Lambda$ and $\Gamma$. Assuming $Y \in \mathbb{R}^{n \times K}$, construction of $Y^TY + \rho I$ and corresponding Cholesky factorization, as the first step in updating $X$, require approximately $nK^2$ and $\frac{1}{3}K^3$ operations, respectively. In our analysis we do not account for matrix (re)assignment operations that can be dealt with via memory pre-allocation.
Algorithm 2 SNMF\textsubscript{ADMM}

\textbf{Input:} Adjacency matrix $A$, penalty parameter $\rho > 0$, stopping threshold $\epsilon$, and initializations for $Y^0, L^0, \Gamma^0, \text{and} \Lambda^0$

\textbf{Output:} Final point-assignment matrix $Z^k$

$k \leftarrow 1$

\textbf{While} $\|X^k - X^{k-1}\|_F + \|Y^k - Y^{k-1}\|_F + \|L^k - L^{k-1}\|_F > \epsilon$:

\hspace{1em} (update primal variable $X$)

\hspace{2em} Find Cholesky factorization of $(Y^{k-1})^T Y^{k-1} + \rho I \rightarrow CC^T$

\hspace{2em} Solve $CJ = (AY^{k-1} + \rho L^{k-1} + \Lambda^{k-1})^T$ for $J$ via forward substitution

\hspace{2em} Solve $C^T (X^k)^T = J$ for $X^k$ via backward substitution

\hspace{1em} (update primal variable $Y$)

\hspace{2em} Find Cholesky factorization of $(X^k)^T X^k + \rho I \rightarrow DD^T$

\hspace{2em} Solve $DH = (AX^k + \rho L^{k-1} + \Gamma^{k-1})^T$ for $H$ via forward substitution

\hspace{2em} Solve $D^T (Y^k)^T = H$ for $Y^k$ via backward substitution

\hspace{1em} (update primal variable $L$)

\hspace{2em} $L^k = \frac{1}{2} \left[ X^k + Y^k - \frac{1}{\rho} (\Lambda^{k-1} + \Gamma^{k-1}) \right]^+$

\hspace{1em} (update dual variable $\Lambda$)

\hspace{2em} $\Lambda^k = \Lambda^{k-1} + \rho (L^k - X^k)$

\hspace{1em} (update dual variable $\Gamma$)

\hspace{2em} $\Gamma^k = \Gamma^{k-1} + \rho (L^k - Y^k)$

$k \leftarrow k + 1$

\textbf{End}

Additionally, whenever possible we take advantage of the symmetry of the matrices involved, as is for example the case when computing $Y^T Y + \rho I$. With the sparse graph structure used in this work (see section 5.1 for more information), the resulting adjacency matrix $A$ has $q = \lceil \log_2 n \rceil + 1$ nonzero entries per row, and therefore computing $AY + \rho L + \Lambda$ requires approximately $(2q + 3) nK$ operations. Considering the $2nK^2$ operations needed for forward and backward substitutions, the total per iteration cost of updating
X (or Y) adds up to \( \frac{1}{3}K^3 + 3nK^2 + 2 (n \log_2 n) K + 5nK \) flops. Updating the primal variable \( L \) can be done using \( 6nK \) basic operations. Together with the \( 3nK \) operations needed for updating each dual variable, the total per iteration cost of SNMF_{ADMM} is given by

\[
\tau_{ADMM} = \frac{2}{3}K^3 + 6nK^2 + 4 (n \log_2 n) K + 22nK.
\] (23)

In practice the number of data points \( n \) greatly exceeds the number of clusters \( K \), and hence the number of flops in (23) can be approximated by \( \tau_{ADMM} \approx 2nK (3K + 2 \log_2 n) \).

For comparison the SymNMF algorithm from (Kuang et al, 2012), a projected Newton-like algorithm for solving (1) (see section 2.3), has comparatively high per iteration computational cost of \( \mathcal{O}(n^3K^3) \). The authors propose a method that takes a limited number of subsampled Hessian evaluations per iteration. This adjustment lowers the per iteration cost of their approach to

\[
\tau_{SymNMF} \approx \mathcal{O}(n^3K),
\] (24)

while retaining something of the quadratic convergence of the standard Newton’s method. However, even such an inexpensive Newton’s approach has serious scaling issues in terms of memory and computation time when dealing with large real world data sets of size \( n = 10,000 \) or more. Moreover, because \( n \) is typically large the per iteration cost of SymNMF greatly surpasses that of SNMF\(_{ADMM}\) derived in (23).

5 Experiments

In this section we present the results of applying our proposed algorithms (SNMF\(_{APG}\) and SNMF\(_{ADMM}\)) to several commonly used benchmark data sets including six synthetic and two real world data sets. In order to evaluate the clustering efficacy of our algorithm we compare it to the standard normalized spectral clustering (Spec) algorithm (Ng et al, 2002), Nonnegative Matrix Factorization (NMF) built in MATLAB which uses the popular alternating least squares solution approach (Berry et al, 2007; Lee and Seung, 2001), and to the Symmetric Nonnegative Matrix Factorization (SymNMF) algorithm (Kuang et al, 2012) discussed in section 2.3. As a stopping condition for both SNMF\(_{APG}\) and SNMF\(_{ADMM}\) algorithms a stopping threshold of \( \epsilon = 10^{-5} \) was used for all experiments. This threshold was achieved for all experiments.
reported here with both algorithms keeping $\rho$ fixed at $\rho = 1$ and $\rho = 0.1$ for SNMF$_{APG}$ and SNMF$_{ADMM}$, respectively. These choices were made by running both algorithms on the two real benchmark datasets 5 times each using $k = 20$ clusters in each instance, as detailed in subsection 5.3, over a set of 20 equally spaced values for $\rho$ in the range $[10^{-2}, 10]$. We then chose the value of $\rho$ for each algorithm that provided the strongest average performance on the two datasets. However we note that the choice of $\rho$ was quite robust over the entire range of tested values in these initial experiments for both algorithms. With each algorithm such a choice for $\rho$ forces the final matrix $L$ and its respective surrogate variables to be extremely similar when the algorithms converge, and thus the final assignment of datapoints in each experiment (and thus the quality of performance) is calculated as with the original SNMF problem (i.e., the $i^{th}$ data point is assigned to the $k^{th}$ cluster where $k$ is the index of the largest entry of the $i^{th}$ row of $L$). All of the experiments in this section were run in MATLAB R2012b on a machine with a 3.40 GHz Intel Core i7 processor and 16 GB of RAM.

5.1 Graph structures

For large-scale and even medium-sized data sets, it is desirable to work with sparse adjacency matrices as they significantly lower the computational time and require less space to store. Therefore, we follow the suggestion in (von Luxburg, 2007; Kuang et al., 2012) and use sparse graphs. The first step in graph-based clustering of a given data set $S = \{d_i | 1 \leq i \leq n\}$, is to address how to construct the adjacency matrix $A$. Following the work in (Kuang et al., 2012), we construct an adjusted $q$-nearest neighbors graph where the $i^{th}$ data point (node) is only connected to its $q$ nearest neighbors denoted by $\mathcal{N}_q(i)$. The matrix $W$ then contains the weights assigned to edges as defined below

$$W_{ij} = \begin{cases} \exp \left( -\frac{||d_i - d_j||^2}{\sigma_i^{(p)} \sigma_j^{(p)}} \right) & j \in \mathcal{N}_q(i) \text{ or } i \in \mathcal{N}_q(j) \\ 0 & \text{otherwise} \end{cases}$$

(25)

Here, the local scale parameter $\sigma_i^{(p)}$ is the distance between $d_i$ and its $p^{th}$ nearest neighbor, where throughout the experiments $p$ is kept fixed to 7. As suggested in (von Luxburg, 2007), the parameter $q$ is chosen as $q = \lceil \log_2 n \rceil + 1$ where $n$ is the total number of data points in the data set $S$. For the sake of comparability of results, we adopt the normalized cut objective
function used in (Kuang et al, 2012) to derive the adjacency matrix $A$ from the weight matrix $W$ via $A = D^{-1/2} W D^{-1/2}$, where $D$ is the diagonal degree matrix associated to $W$.

5.2 Synthetic data sets

We first evaluate our algorithms on six synthetic data sets\(^3\) shown in Figure 1. Each data set is comprised of 3, 4, or 5 clusters of two-dimensional points and the total number of data points vary between 238 (data set 6) and 622 (data set 4). All of the algorithms were run 100 times on each data set with different random initializations for the SNMF factorization matrix $L$. At each run the same initialization was used for SNMF algorithms. Finally, the number of runs at which the algorithms resulted in perfect clustering of each data set is reported in Table 1, as the measure of clustering performance. The best result for each data set is highlighted. Based on the results in Table 1, data sets 5 and 6 can be considered as the most and least challenging data sets, respectively. As can also be seen our algorithms, particularly SNMF\(_{ADMM}\), perform at least as well, and often outperform SymNMF on these synthetic data sets. We do not report the results for NMF and K-means algorithms here since (as expected) both perform very poorly on the types of data sets shown in Figure 1.

| Data Set | Spec | SymNMF | SNMF\(_{APG}\) | SNMF\(_{ADMM}\) |
|----------|------|--------|-----------------|-----------------|
| 1        | 66   | 89     | **90**          | 89              |
| 2        | 87   | 95     | **91**          | **95**          |
| 3        | 61   | 74     | 75              | **80**          |
| 4        | 62   | **84** | 75              | 77              |
| 5        | 37   | 71     | 73              | **80**          |
| 6        | 94   | **100**| **100**         | **100**         |

Table 1: Number of perfect clustering outputs (out of 100) on the synthetic data sets. The highest score for each data set is highlighted.

\(^3\)http://webee.technion.ac.il/~lihi/Demos/SelfTuningClustering.html
5.3 Real world data sets

Recently NMF-based algorithms have been extensively used for clustering tasks, especially for image and document data sets. As representative of image data sets we use the popular COIL-20\textsuperscript{4} data set which contains 1,440 128×128 grayscale images consisting of 20 objects, taken from 72 different viewpoints. Images of the same object then form a cluster, resulting in 20 equally-sized clusters in total. The second real data set used here is Reuters-21578\textsuperscript{5}, a popular text categorization collection consisting of 21,578 documents manually indexed with categories by the personnel from Reuters Ltd. In the original Reuters-21578 data set some documents are assigned more than one label. We remove such documents from the data set so that each remaining document belongs to only one cluster. Moreover, we only keep the largest 20 clusters to avoid having clusters with only a few data points which disrupt the relative balance between clusters’ sizes (these simplifications are commonly made in benchmarking clustering algorithms using this data set).

\textsuperscript{4}http://www.cs.columbia.edu/CAVE/software/softlib/coil-20.php

\textsuperscript{5}http://www.cad.zju.edu.cn/home/dengcai/Data/TextData.html
5.4 Evaluation metric

Upon completion of the cluster assignment process, each cluster is mapped to one of the gold standard classes. Depending on the size of the overlap between each cluster and its mapped class, we can then quantify the efficacy of the clustering algorithm. More formally, let $c_i$ be the cluster label given to the data point $d_i$ by the clustering algorithm, and $g_i$ be the provided gold standard label. The accuracy (AC) score is defined as

$$AC = \frac{\sum_{i=1}^{n} \delta[c_i - g_i]}{n} \times 100,$$

where $\delta[\cdot]$ is the unit impulse sequence which is 1 at zero and 0 everywhere else. Here, we use the Kuhn-Munkres algorithm (Lovasz and Plummer, 2009) to find the best mapping. Note that higher values of AC suggest a better clustering performance, and whenever the clustering and the gold standard are identical, the accuracy reaches its maximum, i.e., $AC = 100$.

5.5 Clustering results

Tables 2 and 3 show the clustering results on the COIL-20 and Reuters-21578 data sets, respectively. In these experiments we randomly select $k$ clusters from the entire data set and run the three clustering algorithms, 5 times each, on the selected clusters. In each of the 5 instances we feed the same random initialization for $L$ to both of our algorithms as well as SymNMF to fairly compare these algorithms. Note that spectral clustering does not require this initialization, and for NMF we use MATLAB’s built-in random initialization. This procedure is repeated 20 times for each $k = 2, 4, 6, \ldots, 14$ for both data sets. The last row in both Tables corresponds to the case where the entire data set is selected ($k = 20$). Since there is only one way to select all clusters, we only report the scores averaged over 5 random initializations of $L$. The computation time reported for all graph-based methods does not include the time spent constructing the neighborhood graph, which for the cases considered here is negligible compared to the runtime of the algorithms themselves. Moreover since both NMF and the graph-based algorithms must be run several times to ensure a good solution is found, this cost is ameliorated even further over the number of runs of each graph-based algorithm.
Table 2: Clustering performance on COIL-20: (top) clustering efficacy in terms of AC score, and (bottom) computation time in seconds.

The best results are again highlighted in bold. As these Tables show, both of our algorithms and particularly SNMF\textsubscript{ADMM}, are highly competitive with the state of the art method (SymNMF) in terms of clustering quality over all experiments. That all graph-based approaches outperform NMF is not surprising given their ability to capture a wider array of cluster configuration, as well as their significant engineering advantage over NMF i.e., they employ a carefully engineered graph transformation of the input data. In terms of total computation time, while spectral clustering demonstrates the lowest computation time on the COIL experiments, SNMF\textsubscript{ADMM} is significantly faster than SymNMF, especially for larger values of $k$. Furthermore on the Reuters-21578 experiments, SNMF\textsubscript{ADMM} is over two orders of magnitude
Table 3: Clustering performance on Reuters-21578: (top) clustering efficacy in terms of AC score, and (bottom) computation time in seconds.

| # of clusters | NMF | Spec | SymNMF | SNMF_{APG} | SNMF_{ADMM} |
|---------------|-----|------|--------|------------|-------------|
| $k = 2$       | 66.80 | 91.56 | **92.88** | 90.56 | 91.46 |
| $k = 4$       | 47.11 | 82.99 | 83.58 | 82.62 | **83.83** |
| $k = 6$       | 34.95 | 64.01 | 73.29 | 71.50 | **73.58** |
| $k = 8$       | 29.31 | 58.58 | 71.26 | 71.00 | **71.76** |
| $k = 10$      | 29.87 | 54.85 | 68.13 | 67.66 | **68.83** |
| $k = 12$      | 26.87 | 51.42 | 68.03 | 67.14 | **68.06** |
| $k = 14$      | 25.39 | 45.73 | 67.05 | 66.79 | **67.29** |
| $k = 20$      | 23.65 | 48.92 | **65.80** | 64.07 | 65.76 |

| # of clusters | NMF | Spec | SymNMF | SNMF_{APG} | SNMF_{ADMM} |
|---------------|-----|------|--------|------------|-------------|
| $k = 2$       | 1.33 | 0.15 | 3.67   | 7.79       | **0.11**    |
| $k = 4$       | 2.53 | 0.23 | 12.74  | 14.15      | **0.22**    |
| $k = 6$       | 8.64 | 0.85 | 104.60 | 81.43      | **0.84**    |
| $k = 8$       | 11.17 | 1.39 | 178.66 | 120.55     | 1.14        |
| $k = 10$      | 11.53 | 1.29 | 197.58 | 121.56     | 1.22        |
| $k = 12$      | 19.53 | 2.57 | 416.22 | 201.20     | **2.18**    |
| $k = 14$      | 23.84 | 2.92 | 566.93 | 258.79     | **2.68**    |
| $k = 20$      | 31.74 | 3.97 | 800.08 | 383.61     | **3.81**    |

faster than SymNMF in a majority of the cases, even outperforming spectral clustering in terms of computation time.

6 Conclusion

In this work, we have introduced two novel algorithms for solving the SNMF problem in (1), an exceptionally strong model for graph-based clustering applications. In particular, the experimental evidence put forth in this work indicates that our algorithms are not only as effective as the state of the art approach, but also in the case of SNMF_{ADMM} that it may run on average one
two orders of magnitude faster than the state of the art SNMF approach in terms of computation time. While we make strong statements regarding the mathematical convergence of SNMF_{ADMM} (see Appendix), proving complete convergence of this algorithm remains an open problem for future work. Thus our two algorithms present an interesting tradeoff between computational speed and mathematical convergence guarantee: SNMF_{APG} is provably convergent yet considerably slower than SNMF_{ADMM}, for which less can be currently said regarding provable convergence. Thus overall the empirical evidence presented here, combined with per iteration complexity analysis and strong proof of mathematical convergence of SNMF_{ADMM}, suggests that our algorithms may extend the practical usability of the SNMF framework to general large-scale clustering problems, a research direction we will pursue in the future.

7 Appendix

7.1 Lipschitz constant for SNMF_{APG}

If a convex function has Lipschitz continuous gradient with constant $T$, then the inverse of this value can be used as a fixed step length for all iterations of (accelerated) proximal gradient (see e.g., (Beck and Teboulle, 2009)). To calculate the Lipschitz constants of $f(L, Z) = \|A - LZ^T\|^2_F + \rho \|L - Z\|^2_F$ in the $L$ and $Z$ directions independently it suffices to compute the maximum eigenvalue of the Hessian in both directions (see e.g., (Watt et al., 2016)).

In the $L$ direction we easily have that Hessian in $L$, denoted as $\nabla^2_L f$, may be written as

$$\nabla^2_L f = Z^T Z + \rho I,$$

where $I$ is the identity matrix of appropriate size. The Lipschitz constant in this instance is then given as the maximum eigenvalue of this matrix, i.e., $T_L = \|Z^T Z + \rho I\|_2$. Likewise in the $Z$ direction the Hessian in $Z$, denoted by $\nabla^2_Z f$, may be written as

$$\nabla^2_Z f = L^T L + \rho I,$$
and the corresponding Lipschitz constant is then given as $T_Z = \|L^T L + \rho I\|_2$.

7.2 Convergence proof of SNMF$_{ADMM}$ to a KKT point

The Lagrangian corresponding to our reformulated SNMF problem in (15) may be written as

$$\mathcal{L}(X, Y, L, \Lambda, \Gamma, \Omega) = \frac{1}{2} \|XY^T - A\|_F^2 + \langle \Lambda, L - X \rangle + \langle \Gamma, L - Y \rangle + \langle \Omega, L \rangle$$

(29)

where $\Omega \leq 0$. The KKT conditions associated to our problem are then given by

$$\begin{align*}
(XY^T - A)Y - \Lambda &= 0 \\
(YX^T - A)X - \Gamma &= 0 \\
\Lambda + \Gamma + \Omega &= 0 \\
X - L &= 0 \\
Y - L &= 0 \\
L &\geq 0 \\
\Omega &\leq 0 \\
\langle \Omega, L \rangle &= 0
\end{align*}$$

(30)

Here the first three equations are given by $\nabla_X \mathcal{L}$, $\nabla_Y \mathcal{L}$, and $\nabla_L \mathcal{L}$, the second three equations enforce primal feasibility, the next dual feasibility, and the final equation ensures complementary slackness holds. Rearranging the third equation allows us to simplify final two lines giving the equivalent KKT system:

$$\begin{align*}
(XY^T - A)Y - \Lambda &= 0 \\
(YX^T - A)X - \Gamma &= 0 \\
X - L &= 0 \\
Y - L &= 0 \\
L &\geq 0 \\
\Lambda + \Gamma &\geq 0 \\
\langle \Lambda + \Gamma, L \rangle &= 0
\end{align*}$$

(31)
Let \( Z \overset{\Delta}{=} (X, Y, L, \Lambda, \Gamma) \) and denote by \( \{Z^k\}_{k=1}^\infty \) the sequence generated by SNMF\(_{ADMM}\) given in algorithm 2. Assuming

\[
\lim_{k \to \infty} (Z^{k+1} - Z^k) = 0
\]  

(32)

then any limit point of \( \{Z^k\}_{k=1}^\infty \) is a KKT point of our reformulation and consequently any limit point of \( \{L^k\}_{k=1}^\infty \) is a KKT point of the original SNMF problem.

Subtracting off the previous iterate from each line of our ADMM algorithm gives the following set of equations

\[
X^{k+1} - X^k = (AY^k + \rho L^k + \Lambda^k) \left( (Y^k)^T Y^k + \rho I \right)^{-1} - X^k
\]

\[
Y^{k+1} - Y^k = (AX^{k+1} + \rho L^k + \Gamma^k) \left( (X^k)^T X^k + \rho I \right)^{-1} - Y^k
\]

\[
L^{k+1} - L^k = \frac{1}{2} \left[ X^{k+1} - \frac{1}{\rho} \Lambda^k + Y^{k+1} - \frac{1}{\rho} \Gamma^k \right]^+ - L^k
\]

\[
\Lambda^{k+1} - \Lambda^k = \rho \left( L^{k+1} - X^{k+1} \right)
\]

\[
\Gamma^{k+1} = \rho \left( L^{k+1} - Y^{k+1} \right)
\]

(33)

Since we have assumed \( Z^{k+1} - Z^k \to 0 \) the left (and consequently right) hand side of each equation above goes to zero. Isolating the right hand side of each and simplifying gives

\[
\left( X^k (Y^k)^T - A \right) Y^k - \Lambda^k = 0
\]

\[
\left( Y^k (X^k)^T - A \right) X^k - \Gamma^k = 0
\]

\[
\frac{1}{2} \left[ X^{k+1} - \frac{1}{\rho} \Lambda^k + Y^{k+1} - \frac{1}{\rho} \Gamma^k \right]^+ - L^k = 0
\]

\[
L^{k+1} - X^{k+1} = 0
\]

\[
L^{k+1} - Y^{k+1} = 0
\]

(34)

From the first and last two equations we can see that the first four KKT conditions are satisfied at any limit point of the ADMM algorithm

\[
\hat{Z} = \left( \hat{X}, \hat{Y}, \hat{L}, \hat{\Lambda}, \hat{\Gamma} \right)
\]

(35)
In particular at such a limit point we have, by construction of the algorithm, that $\hat{L} \geq 0$. Since $\hat{L} = \hat{X} = \hat{Y}$ some simple substitution into the third ADMM equation gives

$$\left[ \hat{L} - \frac{1}{2\rho} (\hat{\Lambda} + \hat{\Gamma}) \right]^+ = \hat{L}$$

(36)

Now if $\hat{L} = 0$ then we have $\left[ - (\hat{\Lambda} + \hat{\Gamma}) \right]^+ = 0$ in which case $\hat{\Lambda} + \hat{\Gamma} \geq 0$. Otherwise, if $\hat{L} > 0$ then it must be the case that $\hat{\Lambda} + \hat{\Gamma} = 0$. This shows at any limit point $\hat{Z}$ that the final KKT conditions ($\hat{\Lambda} + \hat{\Gamma} \geq 0$ and complementary) hold as well. Hence we have shown that the sequence $\{\hat{Z}^k\}_{k=1}^\infty$ indeed converges to a KKT point of the reformulation in (15). The fact that $\{\hat{L}^k\}_{k=1}^\infty$ converges to a KKT point of the original SNMF formulation in (1) follows immediately from equivalence of our reformulation to this problem. This shows that - when convergent - the output of our ADMM algorithm is a KKT point of the original SNMF problem in (1).

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