

Monotonous (Semi-)Nonnegative Matrix Factorization

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Abstract

Nonnegative matrix factorization (NMF) factorizes a non-negative matrix into product of two non-negative matrices, namely a signal matrix and a mixing matrix. NMF suffers from the scale and ordering ambiguities. Often, the source signals can be monotonous in nature. For example, in source separation problem, the source signals can be monotonously increasing or decreasing while the mixing matrix can have nonnegative entries. NMF methods may not be effective for such cases as it suffers from the ordering ambiguity. This paper proposes an approach to incorporate notion of monotonicity in NMF, labeled as *monotonous NMF*. An algorithm based on alternating least-squares is proposed for recovering monotonous signals from a data matrix. Further, the assumption on mixing matrix is relaxed to extend monotonous NMF for data matrix with real numbers as entries. The approach is illustrated using synthetic noisy data. The results obtained by monotonous NMF are compared with standard NMF algorithms in the literature, and it is shown that monotonous NMF estimates source signals well in comparison to standard NMF algorithms when the underlying sources signals are monotonous.

Keywords: Nonnegative matrix factorization, Monotonicity, Unsupervised learning, Blind source separation

1 Introduction

Nonnegative matrix factorization (NMF) is one of the widely used matrix factorization techniques with application areas ranging from basic sciences such as chemistry, environmental science, systems

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biology to image and video processing, blind source separation, text mining, social network analysis [3, 4, 13, 15]. The reasons of wide applicability of NMF are two folds: (i) Non-negativity feature is prevalent in real world data, and (ii) the latent factors estimated by NMF are easily interpretable. Further, the seminal paper by Lee and Seung [9, 10] has helped in popularizing NMF in various fields.

In unsupervised learning methods, the objective is to extract signals or features from the given data. For example, in blind source separation (BSS), the objective is to identify the underlying source signals from noisy data. NMF has been routinely applied to separate source signals from noisy data [3, 14]. NMF decomposes a data matrix into a mixing matrix (coefficients of signals), and a source signal matrix. Since NMF suffers from ordering and scaling ambiguities, NMF factorization is not unique [3, 14]. To obtain appropriate solution, constraint such as sparsity has been incorporated in NMF [3, 6]. Further, semi-NMF imposes non-negativity constraints only on the source signals and allows the mixed sign entries in data and mixing matrices [4].

Many algorithms have been proposed to improve the speed and convergence for NMF. One of the most commonly used algorithms is multiplicative update rules and its variants proposed in [1, 10]. Recently, several algorithms in alternating least-squares framework combined with numerical optimization techniques, active-set method [8], projected gradient methods [11], quadratic programming [16] etc., have been proposed to improve speed and convergence for NMF. Further, necessary and sufficient conditions for unique NMF decomposition have been also investigated [5, 7]. Although there have been considerable work on improvement of algorithms for better solutions, best of our knowledge, there is no attempt on solving monotonicity in signals in NMF.

Source signals in chemistry and systems biology often exhibit monotonous property. In such scenarios, the formulation of monotonicity constraints is important for recovering source signal using NMF or semi-NMF. In this paper, it is proposed to investigate how to resolve monotonicity in NMF. We will propose a new approach, called monotonous NMF, for recovering monotonous source signals from noisy data. Further, we will extend this approach to semi-NMF. Two algorithms for monotonous (semi-) NMF are also proposed. The approach is demonstrated on synthetic data. Moreover, future work on incorporation of sparseness and integer entries in mixing matrix will be discussed.

The rest of this paper is organized as follows. In Section 2, the matrix factorization and NMF related background are introduced. We propose extensions of NMF which resolves monotonicity of source signal in Section 3. Section 4 illustrates monotonous NMF on simulation studies based on synthetic data sets. Further, it compares the performance of the proposed monotonous NMF with two NMF algorithms in the existing literature. Section 5 concludes the paper. Next, the notations used in the paper are described.

1.1 Notations

The bold capital and small letters are used for defining matrices and vectors; the small italic letters are used to define scalar quantities; $\mathbf{w}_{\cdot,i}$ and $\mathbf{h}_{i,\cdot}$ are used for denoting column and row vectors, respectively; $\mathbf{Q}(i,j)$ denotes (i,j) th element of matrix \mathbf{Q} ; $p(\cdot)$ indicates permutations; $\text{vec}(\mathbf{Q})$ indicates the vectorization of a matrix \mathbf{Q} which converts the matrix into a column vector; $(\cdot)^+$ indicates pseudo-inverse of matrix; \mathbf{Q}^T is transpose of matrix \mathbf{Q} ; $\mathbb{R}^{m \times n}$ indicates $m \times n$ -dimensional matrices; $\|\cdot\|$ denotes Frobenius norm; $\|\cdot\|_1$ denotes L_1 -norm of a vector; \mathbb{Z} is integers; \mathbb{R}_+ indicates nonnegative real numbers; \mathbb{S}_+^n denotes $n \times n$ -dimensional symmetric positive semidefinite matrices; \otimes denotes Kronecker products; \mathbf{I}_n is an n -dimensional identity matrix; $\mathbf{0}_n$ denotes vector of length n with zeros as elements; \geq or \leq indicates component-wise inequality for matrices and vectors.

2 Matrix Factorization

A data matrix $\mathbf{Z} \in \mathbb{R}^{n \times m}$ can be factorized as product of $\mathbf{W} \in \mathbb{R}^{n \times s}$ and $\mathbf{H} \in \mathbb{R}^{s \times m}$ for $s \ll \min(m, n)$ as follows:

$$\mathbf{Z} \approx \mathbf{W} \mathbf{H}. \quad (1)$$

In BSS problems, \mathbf{W} is unknown mixing matrix and \mathbf{H} is source signal matrix containing unknown signals. Then, m is the number of observations, n the number of samples, and s is the number of sources. Note that Eq. (1) considers approximate factorization of the data matrix. Since physical systems are often corrupted by noise, the exact factorization of \mathbf{Z} into \mathbf{W} and \mathbf{H} of the data should not be attempted. In presence of noise, the exact factorization of \mathbf{Z} can be written as

$$\mathbf{Z} = \mathbf{W} \mathbf{H} + \mathbf{E}, \quad (2)$$

where \mathbf{E} is an $m \times n$ -dimensional matrix containing a contribution of noise in a given data.

If \mathbf{W} is known and $\text{rank}(\mathbf{W}) = s$, then the least-squares solution of the unknown signal matrix is given by $\hat{\mathbf{H}} = \mathbf{W}^+ \mathbf{Z}$. However, \mathbf{W} is often not known, and the objective of BSS problems is to estimate the unknown mixing matrix and signal matrix from the given data matrix. Note that BSS problems can be also viewed as unsupervised learning methods where the objective is to extract useful features from the given data. To accomplish this task, a prior knowledge about the underlying system such as non-negativity, and sparsity are imposed as constraints. These constraints lead to factorization of the data matrix with meaningful physical insights. The non-negativity constraint leads to popular non-negative matrix factorization (NMF). In the next section, NMF is described briefly.

2.1 Nonnegative matrix factorization (NMF)

NMF aims to factorize the \mathbf{Z} into two nonnegative matrices $\mathbf{W} \in \mathbb{R}_+^{n \times s}$ and $\mathbf{H} \in \mathbb{R}_+^{s \times m}$. In NMF, the following problem is solved to obtain \mathbf{W} and \mathbf{H}

$$\begin{aligned} \min_{\mathbf{W}, \mathbf{H}} \quad & \|\mathbf{Z} - \mathbf{W}\mathbf{H}\| \\ \text{st} \quad & \mathbf{W} \geq \mathbf{0}, \mathbf{H} \geq \mathbf{0}. \end{aligned} \quad (3)$$

The imposing of nonnegative constraints leads to only additive combinations of several rank-one factors to represent the data. Several algorithms have been proposed in the literature to solve Eq. (3), efficiently. However, NMF solution suffers from the following ambiguities [14]:

- Scale ambiguity: Consider a non-singular matrix $\mathbf{T} \in \mathbb{R}_+^{s \times s}$. Then, the factorization of \mathbf{Z} can also be represented as:

$$\mathbf{Z} \approx \mathbf{W}\mathbf{H} = (\mathbf{W}\mathbf{T})(\mathbf{T}^{-1}\mathbf{H}) = \mathbf{W}_T\mathbf{H}_T. \quad (4)$$

Eq. (4) indicates that \mathbf{W}_T and \mathbf{H}_T are also solution of the problem (3). Hence, NMF leads to a local optimum of the solution depending on the initialization, and provides numerous solutions to the problem (3).

- Ordering: Note that $\mathbf{Z} \approx \sum_i \mathbf{w}_{:,i} \mathbf{h}_{i,:} = \sum_i \mathbf{w}_{:,p(i)} \mathbf{h}_{p(i),:}$ with $p(\cdot)$ is an ordering (or permutation). Hence, it is not possible to recover the order of the columns of \mathbf{W} and of the rows \mathbf{H} .

Therefore, the formulation of NMF in Eq. (3) has many solutions. Additional constraints such as sparsity, partial or full knowledge of noisy \mathbf{W} need to be imposed to reduce the number solutions or to obtain a unique solution of the problem (3). These constraints depend on the applications and underlying physical system. Often, the signal sources are in increasing or decreasing orders, i.e., monotonous in nature. In such case, each row of \mathbf{H} contains ordered elements. Hence, the monotonous constraint can be added in the optimization problem (3) for recovering these signals from the data matrix. The main objective of this paper is to develop an approach based on NMF for recovering monotonous signal sources. This leads to a novel method, called monotonous NMF, which is described next.

3 Monotonous NMF

In this section, the monotonous constraints on the source signals will be formulated and imposed on the factorization problem (3). Consider the i th row of \mathbf{H} matrix, $\mathbf{h}_{i,:}$ with $i = 1, \dots, s$, whose elements are monotonously increasing or decreasing order. Without loss of generality, we assume that out of the s rows, the first c rows have entries which are monotonously increasing, while the remaining rows

have entries that are monotonously decreasing. Then, the following relationships hold between the elements:

$$\begin{aligned} h_{k,1} &\leq h_{k,2} \leq \dots \leq h_{k,m}, \quad k = 1, \dots, c, \quad (\text{increasing order}) \\ h_{l,1} &\geq h_{l,2} \geq \dots \geq h_{l,m}, \quad l = c + 1, \dots, s, \quad (\text{decreasing order}). \end{aligned} \quad (5)$$

The optimization problem in Eq. (3) can be reformulated by imposing the constraints in Eq. (5) as:

$$\begin{aligned} &\min_{\mathbf{W}, \mathbf{H}} \|\mathbf{Z} - \mathbf{WH}\| \\ &\text{st } \mathbf{W} \geq \mathbf{0}, \quad \mathbf{H} \geq \mathbf{0}, \\ &h_{k,1} \leq h_{k,2} \leq \dots \leq h_{k,m}, \quad k = 1, \dots, c, \\ &h_{l,1} \geq h_{l,2} \geq \dots \geq h_{l,m}, \quad l = (c + 1), \dots, s. \end{aligned} \quad (6)$$

The formulation in Eq. (6) is nonconvex optimization problem. The solution to the optimization problem (6) can be obtained by decomposing it into two subproblems. These problems can be solved alternately till the solution converges. This approach is known as alternating least squares (ALS) in the literature [8, 11]. The two subproblems can be formulated as follows:

- Given \mathbf{H} :

$$\begin{aligned} &\min_{\mathbf{W}} \|\mathbf{Z} - \mathbf{WH}\| \\ &\text{st } \mathbf{W} \geq \mathbf{0} \end{aligned} \quad (7)$$

- Given \mathbf{W} :

$$\begin{aligned} &\min_{\mathbf{H}} \|\mathbf{Z} - \mathbf{WH}\| \\ &\text{st } \mathbf{H} \geq \mathbf{0} \\ &h_{k,1} \leq h_{k,2} \leq \dots \leq h_{k,m}, \quad k = 1, \dots, c, \\ &h_{l,1} \geq h_{l,2} \geq \dots \geq h_{l,m}, \quad l = (c + 1), \dots, d. \end{aligned} \quad (8)$$

Note that objective functions in Eqs. (7) and (8) are quadratic functions. If we can formulate these subproblems in terms of standard quadratic programming as follows:

$$\begin{aligned} &\min_{\mathbf{x}} \frac{1}{2} \mathbf{x}^T \mathbf{P} \mathbf{x} + \mathbf{f}^T \mathbf{x} \\ &\text{st } \mathbf{G} \mathbf{x} \leq \mathbf{l} \\ &\quad \mathbf{K} \mathbf{x} = \mathbf{r} \end{aligned} \quad (9)$$

where $\mathbf{x} \in \mathbb{R}^p$, $\mathbf{P} \in \mathbb{S}_+^p$, $\mathbf{G} \in \mathbb{R}^{t \times p}$, $\mathbf{l} \in \mathbb{R}^p$, $\mathbf{K} \in \mathbb{R}^{b \times p}$, and $\mathbf{r} \in \mathbb{R}^b$, then it can be shown that both subproblem are convex optimization problems [2]. The standard ALS framework can be applied to solve the problems (7)–(8). We reformulate the problems (7)–(8) in terms of standard form (9) as:

- Given \mathbf{H} :

$$\begin{aligned} & \min_{\mathbf{W}} \text{vec}(\mathbf{W})^T (\mathbf{H}\mathbf{H}^T \otimes \mathbf{I}_n) \text{vec}(\mathbf{W}) - 2 \text{vec}(\mathbf{Z}\mathbf{H}^T)^T \text{vec}(\mathbf{W}) \\ & \text{st} \\ & -\mathbf{I}_{ns} \text{vec}(\mathbf{W}) \leq \mathbf{0}_{ns} \end{aligned} \tag{10}$$

- Given \mathbf{W} :

$$\begin{aligned} & \min_{\mathbf{H}} \text{vec}(\mathbf{H})^T (\mathbf{I}_m \otimes \mathbf{W}^T \mathbf{W}) \text{vec}(\mathbf{H}) - 2 \text{vec}(\mathbf{Z}^T \mathbf{W})^T \text{vec}(\mathbf{H}) \\ & \text{st} \\ & \begin{bmatrix} -\mathbf{I}_{ms} \\ \mathbf{A} \end{bmatrix} \text{vec}(\mathbf{H}) \leq \mathbf{0}_{ms} \end{aligned} \tag{11}$$

where $\mathbf{A} \in \mathbb{R}^{(m-1)s \times ms}$ is matrix having the form

$$\mathbf{A} = \begin{bmatrix} \mathbf{D}_1 & & & \\ & \mathbf{D}_2 & & \\ & & \ddots & \\ & & & \mathbf{D}_s \end{bmatrix}. \text{ The entries not shown in } \mathbf{A} \text{ are zeros. The matrices } \mathbf{D}_k \in \mathbb{R}^{(m-1) \times m}, k = 1, 2, \dots, c \text{ and } \mathbf{D}_l \in \mathbb{R}^{(m-1) \times m}, l = c+1, \dots, s \text{ are defined as follows:}$$

$$\mathbf{D}_k = \begin{bmatrix} 1 & -1 & & & & \\ & 1 & -1 & & & \\ & & \ddots & \ddots & & \\ & & & 1 & -1 & \\ & & & & 1 & -1 \end{bmatrix}$$

$$\mathbf{D}_l = \begin{bmatrix} -1 & 1 & & & & \\ & -1 & 1 & & & \\ & & \ddots & \ddots & & \\ & & & -1 & 1 & \\ & & & & -1 & 1 \end{bmatrix}$$

Note that \mathbf{D}_k and \mathbf{D}_l are Toeplitz matrices with the first rows being $[1 \ -1 \ 0 \ \dots \ 0]$ and $[-1 \ 1 \ 0 \ \dots \ 0]$, respectively.

Since $\mathbf{H} \geq \mathbf{0}$ and $\mathbf{W} \geq \mathbf{0}$, the matrices $(\mathbf{H}\mathbf{H}^T \otimes \mathbf{I}_n)$ and $(\mathbf{I}_m \otimes \mathbf{W}^T \mathbf{W})$ in Eqs. (10) and (11) are positive semi-definite, and of full rank s . Further, both subproblems (10)–(11) are subjected to linear inequality constraints. Hence, the objective problems in (10)–(11) are quadratic programming (QP) of form (9). Consequently, they are convex optimization problems [2]. The optimal solutions of the problems in Eqs. (10)–(11) exist. Standard QP algorithms such as active-set methods, interior-point

methods etc [2, 12] can be used to solve the optimization problems (10)–(11) in the ALS framework. The implementation of these algorithms is available in commercial scientific packages.

Next, we present an algorithm to solve the optimization problems (10)–(11) for estimating \mathbf{W} and \mathbf{H} given \mathbf{Z} . Further, one can impose the upper bounds on the elements of \mathbf{W} and \mathbf{H} based on the data matrix and the underlying physical problem. Algorithm 1 presents an implementation for solving monotonous NMF problem (6) in the ALS framework.

Data: \mathbf{Z} , number of source signals ($s \ll \min(m, n)$)
Result: \mathbf{W} , \mathbf{H}
initialization: $\mathbf{W}_{old}, \mathbf{H}_{old}$;
while $\|\mathbf{W}_{old} - \mathbf{W}_{new}\| \geq tolerance$ *and* $\|\mathbf{H}_{old} - \mathbf{H}_{new}\| \geq tolerance$ **do**
 | read current;
 | $\mathbf{W}_{new} \Leftarrow$ Solution of (10)
 | $\mathbf{H}_{new} \Leftarrow$ Solution of (11)
end
Return $\mathbf{W} = \mathbf{W}_{new}, \mathbf{H} = \mathbf{H}_{new}$

Algorithm 1: Algorithm for Monotonous NMF

In Algorithm 1, \mathbf{H} can be normalized after each iteration. Then, \mathbf{W} has to be scaled in appropriate manner before proceeding to next iteration. Further, note that the subproblem (10) is a standard subproblem in NMF algorithms based on the ALS framework. Then, the multiplicative rules proposed in [1, 10] can also be used to update \mathbf{W} instead of solving the optimization (10) in the ALS framework. It has been shown that the algorithms in the ALS framework (such as Algorithm 1) decrease the function value at each iteration because the ALS framework produces stationary point at each iteration [8, 11]. Hence, Algorithm 1 converges to a solution but note that the convergence speed may be slower.

3.1 Monotonous Semi-NMF

This section demonstrates how idea of monotonous NMF can be extended by relaxing nonnegative constraints on the mixing matrix, \mathbf{W} and \mathbf{Z} . This will allow to apply monotonous NMF to data matrix consisting negative entries. When we relax nonnegative constraints, \mathbf{W} entries can have both positive or negative signs. This kind of NMF is referred as *semi-NMF* in the literature [4]. However, the entries of signal matrix are still nonnegative and monotonous. This relaxation on the mixing matrix allows the non-positive entries in data matrix. The optimization problem (7) can be reformulated without the non-negativity constraints as follows:

$$\min_{\mathbf{W}} \|\mathbf{Z} - \mathbf{W}\mathbf{H}\|. \quad (12)$$

For given \mathbf{H} , Eq. (12) is a least-squares problem, and hence, the analytical update rule can be obtained as

$$\mathbf{W} = \mathbf{Z}\mathbf{H}^T(\mathbf{H}\mathbf{H}^T)^+ \quad (13)$$

In Eq. (13), $\mathbf{H}\mathbf{H}^T$ is positive semidefinite matrix and its inverse (or pseudo-inverse) exists. With this update rule, a modified version of Algorithm 1 is given in Algorithm 2.

Data: \mathbf{Z} , number of source signals ($s \ll \min(m, n)$)

Result: \mathbf{W} , \mathbf{H}

initialization: \mathbf{W}_{old} , \mathbf{H}_{old} ;

while $\|\mathbf{W}_{old} - \mathbf{W}_{new}\| \geq tolerance$ and $\|\mathbf{H}_{old} - \mathbf{H}_{new}\| \geq tolerance$ **do**

 | read current;
 | $\mathbf{W}_{new} \leftarrow \mathbf{Z}\mathbf{H}_{old}^T(\mathbf{H}_{old}\mathbf{H}_{old}^T)^+$
 | $\mathbf{H}_{new} \leftarrow$ Solution of (11)

end

Return $\mathbf{W} = \mathbf{W}_{new}$, $\mathbf{H} = \mathbf{H}_{new}$

Algorithm 2: Algorithm for Semi-NMF

This extension is in line of work done in [4]. Further, Algorithm 2 converges to a solution as we have discussed for Algorithm 1.

4 Illustrative example

In this section, we demonstrate monotonous NMF on synthetic data involving three source signals. We have performed simulation studies for two scenarios: (S1) monotonically increasing source signals, and (S2) mixed monotonous source signals (two increasing signals, one decreasing signal). The noise-free data matrix is constructed in the following manner. Three monotonically source signals are considered as shown in Figures 1 and 2 for Scenarios S1 and S2, respectively. Fifty sample points of signals are available in both scenarios. The mixing matrix of size (8×3) is generated from uniform distribution in the interval $(0,1)$. The noise-free data matrix \mathbf{Z} of size (8×50) is obtained by multiplication of the mixing matrix and signal source matrix. To generate the noisy data, 5% random uniformly distributed noise is added to the noisy-free data. All simulations are performed in MATLAB. For Algorithm 1, "quadprog" function is used to solve the problems (10)-(11).

The following three methods are applied to both scenarios: (i) Monotonous NMF (labeled MNMF), (ii) NMF using multiplicative rules (labeled NNMF) (MATLAB in-built function), and (iii) fast NMF (labeled NMF) algorithm based on active-set methods in [8] with the assumption of three source signals.

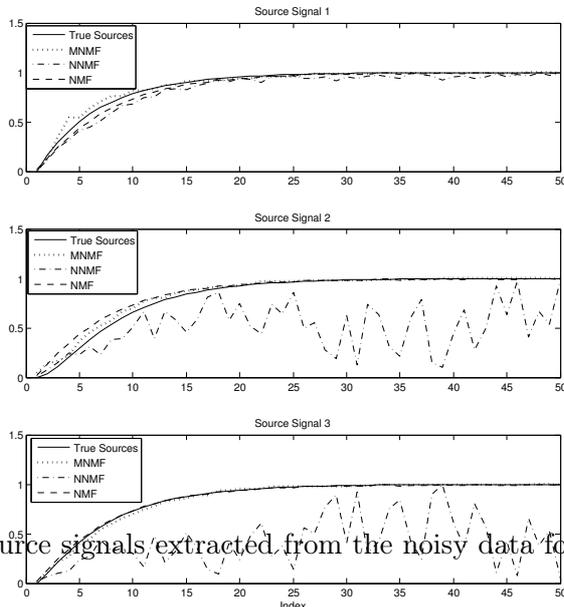


Figure 1: Source signals, extracted from the noisy data for Scenario S1

Scenario S1 The normalized source signals obtained by applying three methods along with the true one are shown in Figure 1 for Scenario S1. The reconstruction errors ($\|\mathbf{Z} - \mathbf{WH}\|$) are 0.1197, 0.1564 and, 0.9835 for MNMF, NNMF, and NMF, respectively. This result shows that MNMF performs well in comparison of NNMF and NMF. It should be noted that NMF estimates rank-deficient source signal matrix ($\text{rank}(\mathbf{H}) = 1$ for NMF). In other words, NMF factorizes the data matrix into single one-rank factor instead of three one-rank factors, while MNMF and NNMF factorize the data matrix into three rank-one factors. However, NNMF fails to capture monotonous behaviour of source signals.

Scenario S2 The normalized source signals obtained using the three methods along with the true one are shown in Figure 2 for Scenario S2. The reconstruction errors ($\|\mathbf{Z} - \mathbf{WH}\|$) are 0.1189, 0.1399 and, 0.5736 for MNMF, NNMF, and NMF, respectively. In this case, MNMF performs better in comparison to other methods to capture both kinds of monotonous signals. In this case, NMF estimates rank-deficient source signal matrix, however, the rank of \mathbf{H} has increased by one rank ($\text{rank}(\mathbf{H}) = 2$ for NMF). Note that NNMF fails to capture monotonous behaviour of source signals in Scenario 2 too.

5 Conclusions

The paper has proposed an approach to incorporate notion of monotonicity in NMF. The new extension is called as monotonous NMF. Monotonous NMF has been applied to recover monotonous source signals from noisy data. Further, we have extended monotonous NMF to semi-NMF by relaxing non-negativity constraints on the mixing matrix. Algorithms for monotonous (semi-)NMF using quadratic

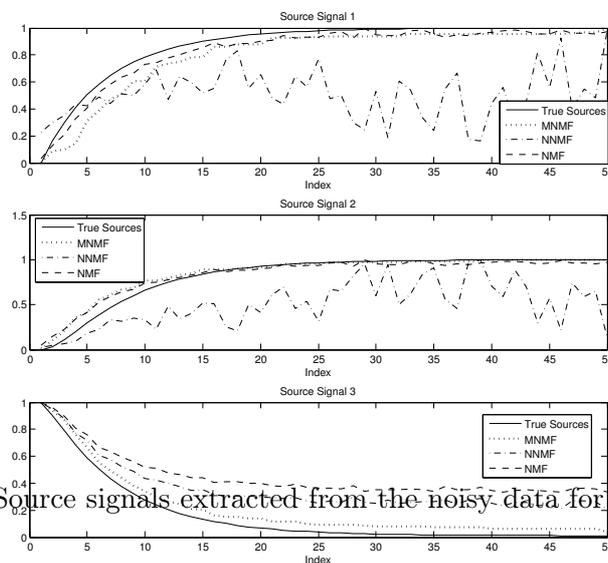


Figure 2: Source signals extracted from the noisy data for Scenario S2

programming have been proposed in the ALS framework. The illustrative examples show that the monotonous NMF performs better in comparison to the algorithms of NMF in the literature when the source signals exhibit monotonous behaviour. This indicates the importance of monotonicity constraint in NMF.

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