Bounded Simplex-Structured Matrix Factorization

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Abstract

In this paper, we propose a new low-rank matrix factorization model dubbed bounded simplex-structured matrix factorization (BSSMF). Given an input matrix $X$ and a factorization rank $r$, BSSMF looks for a matrix $W$ with $r$ columns and a matrix $H$ with $r$ rows such that $X \approx WH$ where the entries in each column of $W$ are bounded, that is, they belong to given intervals, and the columns of $H$ belong to the probability simplex, that is, $H$ is column stochastic. BSSMF generalizes nonnegative matrix factorization (NMF), and simplex-structured matrix factorization (SSMF). BSSMF is particularly well suited when the entries of the input matrix $X$ belong to a given interval; for example when the rows of $X$ represent images, or $X$ is a rating matrix such as in the Netflix and MovieLens data sets where the entries of $X$ belong to the interval $[1,5]$. The simplex-structured matrix $H$ not only leads to an easily understandable decomposition providing a soft clustering of the columns of $X$, but implies that the entries of each column of $WH$ belong to the same intervals as the columns of $W$. In this paper, we first propose a fast algorithm for BSSMF, even in the presence of missing data in $X$. Then we provide identifiability conditions for BSSMF, that is, we provide conditions under which BSSMF admits a unique decomposition, up to trivial ambiguities. Finally, we illustrate the effectiveness of BSSMF on two applications: extraction of features in a set of images, and the matrix completion problem for recommender systems.

Keywords. simplex-structured matrix factorization, nonnegative matrix factorization, identifiability, algorithms.

1 Introduction

Low-rank matrix factorizations have recently emerged as very efficient models for unsupervised learning; see, e.g., [39, 38] and the references therein. The most notable example is principal component analysis (PCA), which can be solved efficiently via the singular value decomposition. In the last 20 years, many new more sophisticated models have been proposed, such as sparse PCA that requires one of the factors to be sparse to improve interpretability [11], robust PCA to handle gross corruption and outliers [7, 6], and low-rank matrix completion, also known as PCA with missing data, to handle missing entries in the input matrix [25].

Among such methods, nonnegative matrix factorization (NMF), popularized by Lee and Seung in 1999 [29], required the factors of the decomposition to be component-wise nonnegative. More precisely, given an input matrix $X \in \mathbb{R}^{m \times n}$ and a factorization rank $r$, NMF looks for a nonnegative matrix $W$ with $r$ columns and a nonnegative matrix $H$ with $r$ rows such that $X \approx WH$. NMF has been shown

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to be useful in many applications, including topic modeling, image analysis, hyperspectral unmixing, and audio source separation; see [9, 13, 16] for more examples. The main advantage of NMF compared to previously introduced low-rank models is that the nonnegativity constraints on the factors $W$ and $H$ lead to an easily interpretable part-based decomposition.

More recently, simplex-structured matrix factorization (SSMF) was introduced as a generalization of NMF [42]; see also [1] and the references therein. SSMF does not impose any constraint on $W$, while it requires $H$ to be column stochastic, that is, $H(:, j) \in \Delta^r$ for all $j$, where $\Delta^r = \{ x \mid x \geq 0, e^\top x = 1 \}$ is the probability simplex and $e$ is the vector of all ones of appropriate dimension. SSMF is closely related to various machine learning problems, such as latent Dirichlet allocation, clustering, and the mixed membership stochastic block model; see [3] and the references therein. Let us recall why SSMF generalizes NMF. Let us normalize the input matrix $X \geq 0$ such that it becomes column stochastic, that is, such that $X^\top e = e$, and let us impose w.l.o.g. that $W$ is column stochastic (by the scaling degree of freedom in the factorization $WH$), that is, $W^\top e = e$. For a decomposition $X = WH$, we have

$$X^\top e = e = (WH)^\top e = H^\top W^\top e = H^\top e,$$

so that $H$ has to be column stochastic.

In this paper, we introduce bounded simplex-structured matrix factorization (BSSMF). BSSMF imposes bounds on the factor $W$, namely $W(i, j) \in [a_i, b_i]$ for all $i, j$ for some parameters $a_i \leq b_i$ for all $i$. For simplicity, given $a \leq b \in \mathbb{R}^m$, we denote the hyper rectangle

$$[a, b] = \{ x \in \mathbb{R}^m \mid a_i \leq x_i \leq b_i \text{ for all } i \},$$

and refer to it as an interval. Let us formally define BSSMF.

**Definition 1 (BSSMF).** Let $X \in \mathbb{R}^{m \times n}$, let $r \leq \min(m, n)$ be an integer, and let $a, b \in \mathbb{R}^m$ with $a \leq b$. The pair $(W, H) \in \mathbb{R}^{m \times r} \times \mathbb{R}^{r \times n}$ is a BSSMF of $X$ of size $r$ for the interval $[a, b]$ if

$$W(:, k) \in [a, b] \text{ for all } k, \quad H \geq 0, \quad \text{and} \quad H^\top e = e.$$

BSSMF reduces to SSMF when $a_i = -\infty$ and $b_i = +\infty$ for all $i$. When $X \geq 0$, BSSMF reduces to NMF when $a_i = 0$ and $b_i = +\infty$ for all $i$, after a proper normalization of $X$; see the discussion around Equation (1).

**Outline and contribution of the paper** The paper is organized as follows. In Section 2, we explain the motivation of introducing BSSMF. In Section 3, we propose an efficient algorithm for BSSMF. In Section 4, we provide an identifiability result for BSSMF, which follows from an identifiability results for NMF. In Section 5, we illustrate the effectiveness of BSSMF on two applications: image feature extraction, and low-rank matrix completion for recommender systems.

**Remark 1 (Extended conference paper).** This paper is an extended version of our conference paper [41]. It provides significant new material:

- A more thorough discussion on the background and the motivations to introduce BSSMF; see Section 2.
- A new algorithm handling missing data and accelerated via data centering; see Section 3.
- Illustrations, examples, and proof for the identifiability of BSSMF; see Section 4.3.
- New numerical experiments on the MNIST and MovieLens data sets; see Sections 3.3 and 5.3.
2 Motivation of BSSMF

The motivation to introduce BSSMF is mostly fourfold; this is described in the next four paragraphs. To illustrate our message, we will rely throughout the paper on two applications:

- Image feature extraction: the entries of \( X \) are pixel intensities. For example, for a gray level image, the entries of \( X \) belong to the interval \([0, 255]\).
- Recommender systems: the entries of \( X \) are ratings of users for some items (e.g., movies). These ratings belong to an interval, e.g., \([1, 5]\) for the Netflix and MovieLens data sets.

Bounded low-rank approximation When the data naturally belongs to intervals, imposing the approximation to belong to the same interval allows to provide better approximations, taking into account this prior information. Such a model, imposing bounds on the approximation, via the element-wise constraints \( a \leq WH \leq b \) for some \( a, b \in \mathbb{R} \), was proposed in [24] and applied successfully to recommender systems. However, this model does not allow to interpret the basis factor, \( W \), in the same way as the data, while it is also difficult to interpret the factor \( H \). In fact, only imposing \( a \leq WH \leq b \) typically leads to dense factors \( W \) and \( H \), which are not easily interpretable.

Another closely related model was proposed in [33] where the entries of the factors \( W \) and \( H \) are required to belong to bounded intervals. The authors showed that their model is suitable for clustering. Nonetheless, it is not clear how to choose the lower and upper bounds on the entries of \( W \) and \( H \) to obtain tight lower and upper bounds for their product \( WH \).

Interpretability Imposing that the entries in \( W \) belong to some interval and that \( H \) is column stochastic resolves the two issues mentioned above, namely boundness and interpretability of the approximation:

- BSSMF implies that the columns of the approximation \( WH \) belong to the same interval as the columns of \( W \). In fact, for all \( j \),
  \[
  X(:,j) \approx WH(:,j) \in [a,b]^m,
  \]
  since \( W(:,k) \in [a,b]^m \) for all \( k \), and the entries of \( H(:,j) \) are nonnegative and sum to one.
- BSSMF allows us to easily interpret both factors: the columns of \( W \) can be interpreted in the same way as the columns of \( X \) (e.g., as movie ratings, or pixel intensities), while the columns of \( H \) provide a soft clustering of the columns of \( X \) as they are column stochastic.

A closely related model is bounded component analysis (BCA) proposed in [10, 12], where the columns of the matrix \( W \) are assumed to belong to compact sets (hyper-rectangle being a special case), while no constraints is imposed on \( H \). Again, without any constraints on \( H \), BCA will generated dense factors which are difficult to interpret. An identifiability theorem is provided in [10, 12] under the strong condition that \( H \) is separable, which requires \( H \) to contain the identity matrix, up to permutation and scaling, as a submatrix. In this paper, we will provide a much weaker condition for identifiability of BSSMF.

BSSMF can be interpreted geometrically similarly as SSMF and NMF: the convex hull of the columns of \( W \), \( \text{conv}(W) \), must contain \( \text{conv}(X) \), since \( X(:,j) = WH(:,j) \) for all \( j \) where \( H \) is column stochastic, while it is contained in the hypercube \([a,b]^m\):

\[
\text{conv}(X) \subseteq \text{conv}(W) \subseteq [a,b]^m.
\]
Identifiability  A drawback of NMF and SSMF is that they are typically not identifiable, without using further constraints. Identifiability is key in practice as it allows to recover the ground truth that generated the data; see the discussion in [13, 26] and the references therein. As we will see in Section 4, BSSMF is identifiable under relatively mild conditions, while it does not require parameter tuning, as opposed to most regularized NMF and SSMF models that are identifiable.

Robustness to overfitting  Another drawback of NMF and SSMF is that they are rather sensitive to the choice of \( r \). When \( r \) is chosen too large, these two models are over-parameterized and will lead to overfitting. This is a well-known behaviour that can be addressed with additional regularization terms that need to be fine tuned [35]. As we will see experimentally in Section 5.3 for matrix completion, without any parameter tuning, BSSMF is much more robust to overfitting than NMF and unconstrained matrix factorization. The reason is that the additional bound constraints on \( W \) prevents columns of \( WH \) to go outside the feasible range, \([a, b]^m\).

3 Inertial block-coordinate descent algorithm for BSSMF

In this paper, we consider the following BSSMF problem

\[
\min_{W, H} g(W, H) := \frac{1}{2} \|X - WH\|_F^2 \quad \text{such that} \quad W(:, k) \in [a, b] \text{ for all } k, H \geq 0, \text{ and } H^\top e = e, \tag{2}
\]

that uses the squared Frobenius norm to measure the error of the approximation.

3.1 Proposed algorithm

Most NMF algorithms rely on block coordinate descent methods, that is, they update a subset of the variables at a time, such that the popular multiplicative updates of Lee and Seung [30], the hieararchical alternating least squares algorithm [8, 18], and a fast gradient based algorithm [20]; see, e.g., [16, Chapter 8] and the references therein for more detail. More recently, an inerTial block majorIzation minimization framework for non-smooth non-convex opTimizAtioN (TITAN) was introduced in [22] and has been shown to be particularly powerful to solve matrix and tensor factorization problems [21, 34, 40].

To solve (2), we therefore apply TITAN which updates one block \( W \) or \( H \) at a time while fixing the value of the other block. In order to update \( W \) (resp. \( H \)), TITAN chooses a block surrogate function for \( W \) (resp. \( H \)), embeds an inertial term to this surrogate function and then minimizes the obtained inertial surrogate function. We have \( \nabla_W g(W, H) = - (X - WH) H^\top \) which is Lipschitz continuous in \( W \) with the Lipschitz constant \( \|HH^\top\| \). Similarly, \( \nabla_H g(W, H) = -W^\top (X - WH) \) is Lipschitz continuous in \( H \) with constant \( \|W^\top W\| \). Hence, we choose the Lipschitz gradient surrogate for both \( W \) and \( H \) and choose the Nesterov-type acceleration as analysed in [22, Section 4.2.1] and [22, Remark 4.1], see also [22, Section 6.1] and [40] for similar applications.

In the case of missing entries in \( X \), let us consider the more general model

\[
\min_{W, H} g(W, H) := \frac{1}{2} \|M \circ (X - WH)\|_F^2 \quad \text{such that} \quad W(:, k) \in [a, b] \text{ for all } k, H \geq 0, \text{ and } H^\top e = e, \tag{3}
\]

where \( \circ \) corresponds to the Hadamard product, and \( M \) is a weight matrix which can model missing entries using \( M(i, j) = 0 \) when \( X(i, j) \) is missing, and \( M(i, j) = 1 \) otherwise. It can also be used in
other contexts; see, e.g., [15, 36, 17]. TITAN can also be used to solve (3), where the gradients are equal to \( \nabla_W g(W, H) = -(M \circ (X - WH))H^\top \) and \( \nabla_H g(W, H) = -W^\top (M \circ (X - WH)) \). We acknowledge that the identifiability result that will be presented in Section 4 does not hold for the case where some data are missing, this is an interesting direction of future research. Algorithm 1 describes TITAN for solving the general problem (3), where \([\cdot]_a^b\) is the column-wise projection on \([a, b]^m\) and \([\cdot]_{\Delta^r}\) is the column-wise projection on the simplex \(\Delta^r\). When some data is missing, the Lipschitz constant of the gradients relatively to \(W\) and \(H\) could be smaller than \(\|HH^\top\|\) and \(\|W^\top W\|\), respectively. Relatively to \(H\) for instance, a smaller Lipschitz constant would be \(\max_i \|W^\top (M; i)e^\top \circ W\|\). We arbitrarily choose to keep \(\|HH^\top\|\) and \(\|W^\top W\|\) even when some data is missing since those values are faster to compute. As proved in [22, Theorem 3.2], Algorithm 1 guarantees a subsequential convergence, that is, every limit point of the generated sequence is a stationary point of Problem (2). The Julia code for Algorithm 1 is available on gitlab\(^1\) (a MATLAB code is also available on gitlab\(^2\) but it does not handle missing data for now).

```
input: Input data matrix \(X \in \mathbb{R}^{m \times n}\), bounds \(a \leq b \in \mathbb{R}^m\), initial factors \(W \in \mathbb{R}^{m \times n}\) s.t. \(W(:, k) \in [a, b]\) for all \(k\) and simplex structured \(H \in \mathbb{R}_+^{r \times n}\), weights \(M \in [0, 1]^{m \times r}\)

output: \(W\) and \(H\)
1. \(\alpha_1 = 1, \alpha_2 = 1, W_{old} = W, H_{old} = H, L^\text{prev}_W = L_W = \|HH^\top\|_2, L^\text{prev}_H = L_H = \|W^\top W\|_2\)
2. repeat
   3. while stopping criteria not satisfied do
      4. \(\alpha_0 = \alpha_1, \alpha_1 = (1 + \sqrt{1 + 4\alpha_0^2})/2\)
      5. \(\beta_W = \min \left[(\alpha_0 - 1)/\alpha_1, 0.9999 \sqrt{L^\text{prev}_W / L_W}\right]\)
      6. \(\bar{W} \leftarrow W + \beta_W(W - W_{old})\)
      7. \(W_{old} \leftarrow W\)
      8. \(W \leftarrow \left[\bar{W} + \frac{(M \circ (X - WH)H^\top)H}{L_W}\right]_a\)
      9. \(L^\text{prev}_W \leftarrow L_W\)
   10. end
11. \(L_H \leftarrow \|W^\top W\|_2\)
12. while stopping criteria not satisfied do
   13. \(\alpha_0 = \alpha_2, \alpha_2 = (1 + \sqrt{1 + 4\alpha_0^2})/2\)
   14. \(\beta_H = \min \left[(\alpha_0 - 1)/\alpha_2, 0.9999 \sqrt{L^\text{prev}_H / L_H}\right]\)
   15. \(\bar{H} \leftarrow H + \beta_H(H - H_{old})\)
   16. \(H_{old} \leftarrow H\)
   17. \(H \leftarrow \left[\bar{H} + \frac{W^\top (M \circ (X - W\bar{H}))}{L_H}\right]_{\Delta^r}\)
   18. \(L^\text{prev}_H \leftarrow L_H\)
19. end
20. \(L_W = \|HH^\top\|_2\)
21 until some stopping criteria is satisfied

Algorithm 1: BSSMF
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\(^1\)https://gitlab.com/vuthanho/bssmf.jl
\(^2\)https://gitlab.com/vuthanho/bounded-simplex-structured-matrix-factorization/
Initialization A simple choice to initialize the factors, \(W\) and \(H\), in Algorithm 1 is to randomly initialize them: for all \(i\), each entry of \(W(i,:)\) is generated using the uniform distribution in the interval \([a_i, b_i]\), while \(H\) is generated using a uniform distribution in \([0, 1]^{r \times n}\) whose columns are then projected on the simplex \(\Delta^r\).

### 3.2 Accelerating BSSMF algorithms via data centering

The BSSMF model is not only invariant to translations of the input data (this is explained in details in Section 4.3), the optimization also is, because of the simplex constraints. In particular, for any \(c \in \mathbb{R}\) and denoting \(J = ee^\top\) the matrix of all ones of appropriate dimension, minimizing

\[
f(W, H) := \frac{1}{2}\|X - WH\|_F^2
\]

or

\[
f_c(W, H) := \frac{1}{2}\|X - cJ - (W - cJ)H\|_F^2,
\]

is equivalent in BSSMF, since \(cJ = cJH\) as \(H\) is column stochastic. However, outside this feasible set, \(f\) and \(f_c\) do not have the same topology. Computing the gradients, we have

\[
\nabla_H f(W, H) = W^\top(WH - X)
\]

which is Lipschitz continuous in \(H\) with the Lipschitz constant \(\|W^\top W\|\), and

\[
\nabla_H f_c(W, H) = W_c^\top(W_cH - X_c)
\]

which is Lipschitz continuous in \(H\) with the Lipschitz constant \(\|W_c^\top W_c\|\), where \(W_c = W - cJ\) and \(X_c = X - cJ\). Particularly, for BSSMF, since \(W\) can be interpreted in the same way as \(X\), we can expect \(\text{mean}(X) \approx \text{mean}(W)\), where \(\text{mean}(\cdot)\) is the empirical mean of the entries of the input. Consequently, if we choose \(c = \text{mean}(X)\), we expect the Lipschitz constant \(\|W^\top_c W_c\|\) to be smaller than \(\|W^\top W\|\). A smaller Lipschitz constant means that, when updating \(H\), the gradient steps are allowed to be larger without losing any convergence guarantee. Hence, with the right translation on our data \(X\), the optimization problem on \(H\) is unchanged on the feasible set but Algorithm 1 can be accelerated.

Let us illustrate this behavior on a small example with \(m = 2, n = 1, r = 2\). We choose \(X = \begin{pmatrix} 0.4 & 0.7 \\ 0.3 & 0.2 \end{pmatrix}\). We fix \(W = \begin{pmatrix} 0.4 & 0.3 \\ 0.7 & 0.2 \end{pmatrix}\) and try to solve both eq. (4) and eq. (5) with respect to \(H\), with \(c = \text{mean}(X)\). We perform 5 projected gradient steps and display the results on Figure 1. On the left, 5 projected gradient steps are performed to update \(H\) based on the original data \(X\). On the right, 5 projected gradient steps are performed to update \(H\) based on the centered data \(X\). The feasible sets (in dash) are exactly the same, and therefore the optimal solutions are also the same. However, we observe that the landscape of the cost function outside the feasible region is smoother when the original data is centered. This allows the solver to converge faster towards the optimal solution, as the gradients point better towards the optimal solution and the stepsizes are larger. The improvement regarding the convergence speed by applying centering with real data will probably not be as drastic as in this small example. Still, minimizing a smoother function is always advantageous, and this will be shown empirically on real data in Section 3.3.

### 3.3 Convergence speed and effect of acceleration strategies on real data

In this subsection, the goal is twofold: (1) show the effect of the extrapolation in TITAN by comparing Algorithm 1 to a non-extrapolated block coordinate descent, and (2) show the acceleration effect of centering the data.

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\(^3\)We empirically noticed that, very often, \(\|W^\top_c W_c\|\) with \(c = \text{mean}(W)\) is of the same order of \(\min_c \|W^\top_c W_c\|\).
Figure 1: Influence of centering the data on the cost function topology regarding $H$ via a small example ($m = 2, r = 2, n = 1$). Left: without centering. Right: with centering. Five projected gradient steps are shown, decomposed through one gradient descent step followed by its projection onto the feasible set.

Figure 2: Evolution of the training error for ml-1m and MNIST, averaged on 10 runs. For ml-1m, $r = 5$, 1 inner iteration. For MNIST, $r = 50$, 10 inner iterations.

We will solve BSSMF for MNIST and ml-1m, these two datasets are properly introduced respectively in Section 5.1 and Section 5.3 in six different scenarios: 3 data related scenarios × 2 algorithmic related scenarios. The data scenarios are raw data, centered data, and data to which a positive offset is added (respectively called ‘plain’, ‘centered’ and ‘uneven’ in Figure 2). Note that ‘uneven’, that is,
adding a positive constant, will worsen the landscape, as \(\|W_c^TW_c\|\) will increase (since \(a \geq 0\)). This scenario will allow to further validate our observation about the acceleration effect of preprocessing. For each data case, 2 algorithms are tested: (1) Alg. 1, and (2) a standard block coordinate descent (BCD) which is Alg. 1 where the \(\beta\)'s are fixed to 0; this corresponds to the popular proximal alternating linearized minimization (PALM) algorithm [5]. When the algorithms are compared on the same data scenario, Alg. 1 always converges faster and to a better solution than BCD. We also observe that when the data is centered, applying the same algorithm always lead to faster convergence than on the plain case. On ml-1m (fig. 2a), applying BCD on the centered data is almost as fast as applying Alg. 1 in the plain case, meaning that a good preprocessing is almost as important as a good acceleration strategy. If we look at the RMSE on the test set, centered data is even more important than a good acceleration strategy. Actually, at the end of the experiment from fig. 2a, on the test set, centered+BCD has a RMSE of 0.91 while plain+Alg. 1 has a RMSE of 0.94. Still on ml-1m, Alg. 1 benefits remarkably from centering the data in comparison to the plain case. We also note an improvement on MNIST (fig. 2b) which is not as noticeable as on ml-1m (probably because this problem is less difficult to solve, which is corroborated by the number of iterations required to converge). Here, the uneven case is just shown to remind that the data points cloud position is of much concern and should not be neglected. Globally, regardless of the dataset, applying Alg. 1 on centered data is the best strategy. As a consequence, it will be our default choice for the experiments in Section 5.

4 Identifiability

Let us first define a factorization model.

**Definition 2** (Factorization model). Given a matrix \(X \in \mathbb{R}^{m \times n}\), and an integer \(r \leq \min(m, n)\), a factorization model is an optimization model of the form

\[
\min_{W \in \mathbb{R}^{m \times r}, H \in \mathbb{R}^{r \times n}} g(W, H) \quad \text{such that} \quad X = WH, W \in \Omega_W, \text{ and } H \in \Omega_H, \tag{6}
\]

where \(g(W, H)\) is some criterion, and \(\Omega_W\) and \(\Omega_H\) are the feasible sets for \(W\) and \(H\), respectively.

Let us define the identifiability of a factorization model, and essential uniqueness of a pair \((W, H)\).

**Definition 3** (Identifiability / Essential uniqueness). Let \(X \in \mathbb{R}^{m \times n}\), and \(r \leq \min(m, n)\) be an integer. Let \((W, H)\) be a solution to a given factorization model (6). The pair \((W, H)\) is essentially unique for the factorization model (6) of matrix \(X\) if and only if any other pair \((W', H')\) \(\in \mathbb{R}^{m \times r} \times \mathbb{R}^{r \times n}\) that solves the factorization model (6) satisfies, for all \(k\),

\[
W'(:, k) = \alpha_k W(:, \pi(k)) \quad \text{and} \quad H'(k, :) = \alpha_k^{-1} H(\pi(k), :),
\]

where \(\pi\) is a permutation of \(\{1, 2, \ldots, r\}\), and \(\alpha_k > 0\) for all \(k\). In other terms, \((W', H')\) can only be obtained as a permutation and scaling of \((W, H)\). In that case, the factorization model is said to be identifiable for the matrix \(X\).

A key question in theory and practice is to determine conditions on \(X\), \(g\), \(\Omega_W\) and \(\Omega_H\) that lead to identifiable factorization models; see, e.g., [13, 26] for discussions.

In the next three sections, we discuss the identifiability of SSMF, NMF, and BSSMF.
4.1 Simplex-structured matrix factorization (SSMF)  

Without further requirements, SSMF is never identifiable; which follows from a result for semi-NMF which is a factorization model than requires only one factor, $H$, to be nonnegative [19]. Let $X = WH$ be an SSMF of $X$. We can obtain other SSMF of $X$ using the following transformation: for any $\alpha \geq 0$, let 

$$W(\alpha) := W\left(\frac{1}{1 + \alpha} I - \frac{\alpha}{r} ee^\top\right),$$

and 

$$H(\alpha) := \left(\frac{1}{1 + \alpha} I + \frac{\alpha}{1 + \alpha} ee^\top\right) H, $$

where $I$ is the identity matrix of appropriate dimension, and the last equality follows from $e^\top H = e^\top$. The matrix $H(\alpha)$ is column stochastic since $H$ and $ee^\top$ are. One can check that $(W(\alpha), H(\alpha))$ is not a permutation and scaling of $(W, H)$ for $\alpha > 0$, while $WH = W(\alpha)H(\alpha)$ since

$$A(\alpha) := \left(\frac{1}{1 + \alpha} I - \frac{\alpha}{r} ee^\top\right)^{-1} = \frac{1}{1 + \alpha} I + \frac{\alpha}{1 + \alpha} ee^\top.$$

Geometrically, to obtain $W(\alpha)$, the columns of $W$ are moved towards the exterior of $\text{conv}(W)$ and hence the convex hull of the column of $W(\alpha)$ contains the convex hull of the columns of $W$ and hence contains $\text{conv}(X)$. This follows from the fact that $W = W(\alpha)A(\alpha)$, where $A$ is column stochastic.

To obtain identifiability of SSMF, one needs either to impose additional constraint on $W$ and/or $H$ such as sparsity [1], or look for a solution minimizing a certain function $g$. In particular, the solution $(W, H)$ that minimizes the volume of the convex hull of the columns of $W$ (see Theorem 1 below for a formula) is essentially unique given that $H$ satisfies the so-called sufficiently scattered condition (SSC). The SSC is defined as follows.

Definition 4 (Sufficiently scattered condition). The matrix $H \in \mathbb{R}^{r \times n}_+$ is sufficiently scattered if the following two conditions are satisfied:

[SSC1] $C = \{x \in \mathbb{R}^r_+ \mid e^\top x \geq \sqrt{r - 1}\|x\|_2\} \subseteq \text{cone}(H)$.

[SSC2] There does not exist any orthogonal matrix $Q$ such that $\text{cone}(H) \subseteq \text{cone}(Q)$, except for permutation matrices. (An orthogonal matrix $Q$ is a square matrix such that $Q^\top Q = I$.)

SSC1 requires the columns of $H$ to contain the cone $C$, which is tangent to every facet of the nonnegative orthant; see Figure 3. Hence it requires some degree of sparsity in $H$. SSC2 is a mild regularity condition which is typically satisfied when SSC1 is satisfied. For more discussions on the SSC, we refer the interested reader to [13] and [16, Chapter 4.2.3], and the references therein.

Theorem 1. [14, 32] The minimum-volume SSMF factorization model,

$$\min_{W \in \mathbb{R}^{m \times r}, H \in \mathbb{R}^{r \times n}} \det(W^\top W) \quad \text{such that} \quad H \geq 0, H^\top e = e,$$

is identifiable for $X = W^2 H^2$ if the pair $(W^2, H^2) \in \mathbb{R}^{m \times r} \times \mathbb{R}^{r \times n}$ satisfies $\text{rank}(W^2) = r$ and $H^2$ is sufficiently scattered.

This is an invertible M-matrix, with positive diagonal elements and negative off-diagonal elements, whose inverse is nonnegative [4].


Figure 3: Illustration of the SCC in three dimensions. On the left: the sets $\Delta^3$ and $C$, they intersect at $(0,0.5,0.5)$, $(0.5,0,0.5)$, and $(0.5,0.5,0)$. (This left figure is similar to [23, Figure 2] and we are grateful to the authors for providing us with the code to generate it.) On the right: examples of a matrix $H \in \mathbb{R}^{3 \times n}$ satisfying the SSC (left), and not satisfying the SSC (right). The left (resp. right) figure is adapted from [23] (resp. [1]).

Note that this result has been generalized to other sets as the probability simplex for the columns of $H$; see [37]. In practice, because of noise and model misfit, optimization models need to balance the data fitting term which measures the discrepancy between $X$ and $WH$, and the volume regularization for $\text{conv}(W)$. This requires the tuning of some parameter, which is a nontrivial process [2, 43].

4.2 Nonnegative matrix factorization (NMF)

As opposed to SSMF, NMF decompositions can be identifiable without the use of additional requirements. One of the most relaxed sufficient condition for identifiability is based on the SSC.

**Theorem 2.** [23, Theorem 4] If $W^\top \in \mathbb{R}^{r \times m}$ and $H \in \mathbb{R}^{r \times n}$ are sufficiently scattered, then the Exact NMF $(W, H)$ of $X = WH$ of size $r = \text{rank}(X)$ is essentially unique.

In practice, it is not likely for both $W^\top$ and $H$ to satisfy the SSC. Typically $H$ will satisfy the SSC, as it is typically sparse. However, in many applications, $W^\top$ will not satisfy the SSC; in particular in applications where $W$ is not sparse, e.g., in hyperspectral unmixing, recommender systems, or imaging. This is why regularized NMF models have been introduced, including sparse and minimum-volume NMF. We refer the interested reader to [16, Chapter 4] for more details.

4.3 Bounded simplex-structured matrix factorization (BSSMF)

A main motivation to introduce BSSMF is that it is identifiable under weaker conditions than NMF. We now state our main identifiability result for BSSMF, it is a consequence of the identifiability result of NMF and the following simple observation: $X = WH$ is a BSSMF for the interval $[a, b]$ implies that $be^\top - X = (be^\top - W)H$ and $X - ae^\top = (W - ae^\top)H$ are Exact NMF decompositions.

**Theorem 3.** Let $W \in \mathbb{R}^{m \times r}$ and $H \in \mathbb{R}^{r \times n}$ satisfy $W(:, k) \in [a, b]$ for all $k$ for some $a \leq b$, $H \geq 0$, and $H^\top e = e$. If $(W - ae^\top)^\top \in \mathbb{R}^{m \times 2m}$ and $H \in \mathbb{R}^{r \times n}$ are sufficiently scattered, then the BSSMF $(W, H)$ of $X = WH$ of size $r = \text{rank}(X)$ for the interval $[a, b]$ is essentially unique.
Proof. Let \((W, H)\) be a BSSMF of \(X\) for the interval \([a, b]\). As in the proof of Lemma 2, we have

\[
X - ae^\top = WH - ae^\top = (W - ae^\top)H,
\]

since \(e^\top = He^\top\). This implies that \((W - ae^\top, H)\) is an Exact NMF of \(X - ae^\top\), since \(W - ae^\top\) and \(H\) are nonnegative. Similarly, we have

\[
be^\top - X = be^\top - WH = (be^\top - W)H,
\]

which implies that \((be^\top - W, H)\) is an Exact NMF of \(be^\top - X\), since \(be^\top - W \geq 0\). Therefore, we have the Exact NMF

\[
\begin{pmatrix}
X - ae^\top \\
be^\top - X
\end{pmatrix} =
\begin{pmatrix}
W - ae^\top \\
be^\top - W
\end{pmatrix}H.
\]

By Theorem 2, this Exact NMF is unique if \((W - ae^\top, H)\) satisfies the SSC. This proves the result: in fact, the derivations above hold for any BSSMF of \(X\). Hence, if \((W, H)\) was not an essentially unique BSSMF of \(X\), there would exist another Exact NMF of \((W - ae^\top, H)\), not obtained by permutation and scaling of \((W - ae^\top, H)\), a contradiction.

The condition that \((W - ae^\top, H)\) is SSC is much weaker than requiring \(W^\top\) to be SSC in NMF. For example, in recommender systems, with \(W(i,j) \in [1, 5]\) for all \((i,j)\), many entries of \(W\) are expected to be equal to 1 or to 5 (the minimum and maximum ratings), so that \((W - ae^\top, H)\) will be sparse, and hence likely to satisfy the SSC. On the other hand, \(W\) is positive, and hence will not admit an essentially unique Exact NMF.

Let us illustrate the difference between NMF and BSSMF on a simple example.

**Example 1** (Non-unique NMF vs. unique BSSMF). Let \(\omega \in [0, 1)\) and let

\[
A_\omega = \begin{pmatrix}
\omega & 1 & 1 & \omega & 0 & 0 \\
1 & \omega & 0 & 0 & \omega & 1 \\
0 & 0 & \omega & 1 & 1 & \omega
\end{pmatrix}.
\]

For \(\omega < 0.5\), \(A_\omega\) satisfies the SSC, while it does not for \(\omega \geq 0.5\); see [27, Example 3], [23, Example 2], [16, Example 4.16]. Let us take

\[
H = 3A_{1/3} = \begin{pmatrix}
1 & 3 & 3 & 1 & 0 & 0 \\
3 & 1 & 0 & 0 & 1 & 3 \\
0 & 0 & 1 & 3 & 3 & 1
\end{pmatrix},
\]

which satisfies the SSC, and

\[
W = 3A_{2/3}^\top = \begin{pmatrix}
2 & 3 & 3 & 2 & 0 & 0 \\
3 & 2 & 0 & 0 & 2 & 3 \\
0 & 0 & 2 & 3 & 3 & 2
\end{pmatrix}^\top,
\]

which does not satisfy the SSC, but has some degree of sparsity. The NMF of

\[
X = WH = \begin{pmatrix}
11 & 9 & 6 & 2 & 3 & 9 \\
9 & 11 & 9 & 3 & 2 & 6 \\
3 & 9 & 11 & 9 & 6 & 2 \\
2 & 6 & 9 & 11 & 9 & 3 \\
6 & 2 & 3 & 9 & 11 & 9 \\
9 & 3 & 2 & 6 & 9 & 11
\end{pmatrix}
\]
is not essentially unique. For example,

\[
X = \begin{pmatrix}
0 & 3 & 1 \\
1 & 3 & 0 \\
3 & 1 & 0 \\
3 & 0 & 1 \\
1 & 0 & 3 \\
0 & 1 & 3
\end{pmatrix}
\begin{pmatrix}
0 & 2 & 3 & 3 & 2 & 0 \\
3 & 3 & 2 & 0 & 0 & 2 \\
2 & 0 & 0 & 2 & 3 & 3
\end{pmatrix}
\]

is another decomposition which cannot be obtained as a scaling and permutation of \((W,H)\).

However, the BSSMF of \(X\) is unique, taking \(a_i = 0\) and \(b_i = 3\) for all \(i\). In fact, \((3-W)^\top\) satisfies the SSC, as it is equal to \(3A_{1/3}\), up to permutation of its columns:

\[
3 - W^\top = \begin{pmatrix}
1 & 0 & 0 & 1 & 3 & 3 \\
0 & 1 & 3 & 3 & 1 & 0 \\
3 & 3 & 1 & 0 & 0 & 1
\end{pmatrix} = 3A_{1/3}(; [4, 5, 6, 1, 2, 3]).
\]

Therefore, by Theorem 3, the BSSMF of \(X\) is unique.

**Scaling ambiguity**  BSSMF is in fact more than essentially unique in the sense of Definition 3. In fact, the scaling ambiguity can be removed because of \(H\) being simplex structured, as shown in the following lemma.

**Lemma 1.** Let \(H \in \mathbb{R}^{r \times n}\) such that \(e^\top H = e^\top\) and \(\text{rank}(H) = r\). Let \(D \in \mathbb{R}^{r \times r}\) be a diagonal matrix, and let \(H' = DH\) be a scaling of the rows of \(H\), and such that \(e^\top H' = e^\top\). Then \(D\) must be the identity matrix, that is, \(D = I\).

**Proof.** Let us denote \(H^\top \in \mathbb{R}^{n \times r}\) the right inverse of \(H\), which exists and is unique since \(\text{rank}(H) = r\), so that \(HH^\top = I\). We have

\[
e^\top H' = e^\top DH = e^\top \\
\Rightarrow e^\top DHH^\top = e^\top H^\top = e^\top\quad\text{since }e^\top H^\top = e^\top HH^\top = e^\top \\
\Rightarrow e^\top D = e^\top\quad\Rightarrow\quad D = I.
\]

Note that this lemma does not require \(H\), \(H'\) and \(D\) to be nonnegative.

**Geometric interpretation of BSSMF**  Solving NMF is equivalent to finding a cone with \(r\) rays in the nonnegative orthant that reconstructs as well as possible the data points. Solving BSSMF is equivalent to finding a polytope with \(r\) vertices within the parallelotope defined by \([a,b]^m\) that reconstructs as well as possible the data points. The fact that BSSMF is constrained within a parallelotope makes BSSMF more constrained, and hence more likely to be essentially unique. This will be illustrated empirically in Section 5.2. Let us provide a toy example to better understand the distinction between NMF and BSSMF, namely let us use Example 1 with \(W = \frac{3}{10}A_{2/3}\) and \(H = \frac{2}{3}A_{1/2}\) so that \(X = WH\) is column stochastic. Figure 4 represents the NMF and BSSMF (for \(a = 0\) and \(b = 3/10\)) problems in a two-dimensional space within the affine hull of \(W\); see [16] for the details on how to construct such a representation. For this rank-3 factorization problem, solving NMF and BSSMF is equivalent to finding a triangle nested between the convex hull of the data points and the corresponding feasible
Figure 4: A geometrical interpretation of BSSMF. Any triangle in the gray filled area containing the data points is a rank-3 solution for NMF. On the contrary, there is a unique rank-3 solution for BSSMF since there is a unique triangle containing the data points in the BSSMF feasible set.

Intuitively, for the BSSMF of $X = WH$ to be essentially unique, $W$ must contain sufficiently many entries equal to the lower and upper bounds, while $H$ must be sufficiently sparse. In practice, it may be beneficial to preprocess the input matrix so that as many entries of $X$ as possible are equal to the lower and upper bounds. In fact, let $X(i, j) = a_i$ for some $i, j$ (a similar observation holds when $X(i, j) = b_j$). Since $X(i, j) = W(i, :)H(:, j)$, $W(i, :) \geq a_i$ and $H(:, j) \in \Delta^r$, we have $W(i, k) = a_i$ for any $k$ such that $H(k, j) > 0$. For example, when each row of $X$ correspond to an image (see Section 5.1 for more details and numerical examples), it is useful to preprocess each row of $X$ so that it belongs to the interval $[0, 1]$, using the preprocessing

$$X(i, :) \leftarrow \frac{X(i, :) - a_i}{b_i - a_i}.$$  

where $a_i = \min_j X(i, j)$, and $b_i = \max_j X(i, j)$. Then $X$ can be approximated with a BSSMF for the interval $[0, 1]^m$.

Interestingly, in the exact case, that is, when $X = WH$, we can assume w.l.o.g. that $[a_i, b_i] = [0, 1]$ for all $i$ in BSSMF.

**Lemma 2.** Let $a \in \mathbb{R}^m$ and $b \in \mathbb{R}^m$ be such that $a_i < b_i$ for all $i$. The matrix $X = WH$ admits a BSSMF for the interval $[a, b]$ if and only if the matrix $\frac{[X - ae^r]}{[b - a)e^r]}$ admits a BSSMF for the interval $[0, 1]^m$, where $\frac{[\cdot]}{[\cdot]}$ is the component-wise division two matrices of the same size.
Proof. Let us show the direction ⇒, the other is obtained exactly in the same way. Let the matrix $X = WH$ admit a BSSMF for the interval $[a, b]$. We have

$$X - ae^\top = WH - ae^\top = (W - ae^\top)H,$$

since $e^\top H = e^\top$, as $H$ is column stochastic. This shows that $X' = X - ae^\top$ admits a BSSMF for the interval $[0, b - a]$ since $W' = (W - ae^\top) \in [0, b - a]$. For simplicity, let us denote $c = b - a > 0$. We have $X' = W'H$, while

$$\frac{[X - ae^\top]}{[(b-a)e^\top]} = \frac{[X']}{[ce^\top]} = \frac{[W'H]}{[ce^\top]} = \frac{[W']}{{ce}^\top}H,$$

because $H$ is column stochastic. In fact, for all $i, j$,

$$\frac{[W'H]_{i,j}}{[ce^\top]_{i,j}} = \sum_k \frac{W'(k, i)H(k, j)}{c_i} = \frac{\sum_k W'(k, i)}{c_i} H(k, j) = \left(\frac{[W']}{[ce^\top]}H\right)_{i,j}.$$

Hence $\frac{[X - ae^\top]}{[(b-a)e^\top]}$ admits a BSSMF for the interval $[0, 1]^m$ since $H$ is column stochastic, and all columns of $\frac{[W']}{[ce^\top]} = \frac{[W - ae^\top]}{[(b-a)e^\top]}$ belong to $[0, 1]^m$. \qed

Remark 2 (What if $a_i = b_i$ for some $i$?). Lemma 2 does not cover the case $a_i = b_i$ for some $i$. In that case, we have $W(i, :) = a_i = b_i$ and therefore $X(i, :) = W(i, :)H = a_i e^\top = b_i e^\top$. This is not an interesting situation, and rows of $X$ with identical entries can be removed. In fact, after the transformation $X - ae^\top$, these rows are identically zero.

Lemma 2 highlights another interesting property of BSSMF: as opposed to NMF, it is invariant to translations of the entries of the input matrix, given that $a$ and $b$ are translated accordingly. For example, in recommender systems data sets such as Netflix and MovieLens, $X(i, j) \in \{1, 2, 3, 4, 5\}$ for all $i, j$. Changing the scale, say to $\{0, 1, 2, 3, 4\}$, does not change the interpretation of the data, but will typically impact the NMF solution significantly\(^5\), while the BSSMF solution will be unchanged, if the interval is translated from $[1, 5]$ to $[0, 4]$ since $H$ is invariant by translation on $X$. This property is in fact coming from SSMF.

5 Numerical experiments

The goal of this section is to highlight the motivation points mentioned in Section 2 on real data sets. All experiments are run on a PC with an Intel(R) Core(TM) i7-9750H CPU @ 2.60GHz and 16GiB RAM. Let us recall that in order to retrieve NMF from Algorithm 1, the bounds need to be set to $(a, b) = (0, +\infty)$ and the projection step on the probability simplex in line 17 should be replaced by a projection on the nonnegative orthant. Hence, in our experiments, both NMF and BSSMF are solved with the same code implementation.

5.1 Interpretability

When applied on a pixel-by-image matrix, NMF allows to automatically extract common features among a set of images. For example, if each row of $X$ is a vectorized facial image, the rows of $W$ will correspond to facial features [29].

\(^5\)In fact, for NMF, it would make more sense to work on the data sets translated to $[0, 4]$, as it would potentially allow it to be identifiable: zeros in $X$ imply zeros in $W$ and $H$, which are therefore more likely to satisfy the SSC.
Let us compare NMF with BSSMF on the widely use MNIST handwritten digits dataset (60,000 images, 28 × 28 pixels) [28]. Each column of X is a vectorized handwritten digit. For BSSMF to make more sense, we preprocess X so that the intensities of the pixels in each digit belong to the interval [0, 1] (first remove from X(:, j) its minimum entry, then divide by the maximum entry minus the minimum entry).

Let us take a toy example with \( n = 500 \) randomly selected digits and \( r = 10 \), in order to visualize the natural interpretability of BSSMF. Fig. 5a shows the features learned by NMF which look like parts of digits. On the other hand, the features learned by BSSMF in Fig. 5b look mostly like real digits, because of the bound constraint and the sum-to-one constraints. We distinguish numbers (like 7, 3 and 6). From a clustering point of view, this is of much interest because a column of H which is near a ray of the probability simplex can directly be associated with the corresponding digit from W. In this toy example, due to \( r \) being small, an 8 cannot be seen. Nonetheless, an eight can be reconstructed as the weighted sum of the representations of a 5, a 3 and an italic 1; see Fig. 6 for an example. Note that since BSSMF is more constrained than NMF, its reconstruction error might be larger than that of NMF. For our example (\( r = 10 \)), BSSMF has relative error \( \|X - WH\|_F/\|X\|_F \) of 61.56%, and NMF of 59.04%. Note that we also compute NMFs using Algorithm 1 where the projections are performed on the nonnegative orthant, instead of on the bounded set for W and on the probability simplex for H. The stopping criteria in line 21, 3 and 12 of Algorithm 1 are a maximum number of iterations equal to 500, 20 and 20, respectively, for both algorithms.

### 5.2 Identifiability

As it is NP-hard to check the SSC [23], we will perform an experiment where only a necessary condition for SSC1 is verified, namely [16, Alg. 4.2]. To see when H satisfies this condition, we first vary \( n \) from 100 to 300 for \( m \) fixed (=28×28). For \( W^T \), we fix \( n \) to 300, and downscale the resolution \( m \) from 28×28 to 12×12 with a linear interpolation (imresize3 in MATLAB), and the rank \( r \) is varied from...
12 to 30. Recall that both factors need to satisfy the SSC to correspond to an essentially unique factorization. In Fig. 7a, we see that $W^\top$ of NMF often satisfies the necessary condition. This is due to NMF learning “parts” of objects [29], which are sparse by nature, and sparse matrices are more likely to satisfy definition 4. On the contrary, even for a relatively large $n$, $H$ is too dense to satisfy the necessary condition. For $r \geq 30$, the factor $H$ generated by NMF never satisfies the condition. Meanwhile, in Fig. 7b we see that $H$ of BSSMF always satisfies the condition when $n \geq 225$ for $r = 30$ and more generally, if $n$ and $m$ are large enough, both $H$ and $(e e^\top - W)^\top$ satisfy the necessary condition. This substantiates that BSSMF provides essentially unique factorizations more often than NMF does.

Figure 7: Ratio, over 10 runs, of the factors generated by NMF in Fig. 7a and by BSSMF in Fig. 7b that satisfy the necessary condition for SSC1 (white squares indicate that all matrices meet the necessary condition, black squares that none do).

5.3 Robustness to overfitting

In this section we compare unconstrained matrix factorization (MF), NMF and BSSMF on the matrix completion problem; more precisely, on rating datasets for recommendation systems. Let $X$ be an item-by-user matrix and suppose that user $j$ has rated item $i$, that rating would be stored in $X_{i,j}$. The matrix $X$ is then highly incomplete since a user has typically only rated a few of the items. In this context, NMF looks for nonnegative factors $W$ and $H$ such that $M \circ X \approx M \circ (WH)$, where $M_{i,j}$ is equal to 1 when user $j$ rated item $i$ and is equal to 0 otherwise. A missing rating $X_{i,j}$ is then estimated by computing $W(i,:)H(:,j)$. Features learned by NMF on rating datasets tends to be parts of typical users. Yet, the nonnegative constraint on the factors hardly makes the features interpretable by a practitioner. Suppose that the rating a user can give is an integer between 1 and 5 like in many rating systems, NMF can learn features whose values may fall under the minimum rating 1 or may exceed the maximum rating 5. Consequently, the features cannot directly be interpreted as typical users. On the contrary, with BSSMF, the extracted features will directly be interpretable if the lower and upper bounds are set to the minimum and maximum ratings. On top of that, BSSMF is expected to be less sensitive to overfitting than NMF since its feasible set is more constrained.

This last point will be highlighted in the following experiment on the ml-1m dataset\(^6\), which contains 1 million ratings from 6040 users on 3952 movies. As in [31], we split the data in two sets: a training set and a testing set. The testing set contains 500 users. We also remove any movie

\(^6\)https://grouplens.org/datasets/movielens/1m/
that has been rated less than 5 times. For the testing set, 80% of a user’s ratings are considered as known. The remaining 20% are kept for evaluation. During the training, we learn W only on the training set. During the testing, the learned W is used to predict those 20% kept ratings of the testing set by solving the $H$ part only on the 80% known ratings. This simulates new users that were not taken into account during the training, but for whom we would still want to predict the ratings. The reported root-mean-square errors (RMSEs) are computed on the 20% kept ratings of the testing set.

In order to challenge the overfitting issue, we vary $r$ in $\{1, 5, 10, 20, 50, 100\}$ for BSSMF, NMF and an unconstrained MF which are all computed using Algorithm 1, where the projections onto the feasible sets are adapted accordingly (projection onto the nonnegative orthant for NMF, no projection for unconstrained MF). The stopping criteria in line 21, 3 and 12 of Algorithm 1 are a maximum number of iterations equal to 200, 1 and 1, respectively, for all algorithms. The experiment is conducted on 10 random initializations and the average RMSEs are reported in Table 1. As expected, BSSMF and NMF are more robust to overfitting than unconstrained MF. Additionnally, BSSMF is also clearly more robust to overfitting than NMF. Its worse RMSE is 0.89 with $r = 100$ (and it is still equal to 0.89 with $r = 200$), while, for NMF, the RMSE is 0.92 when $r = 100$ (which is worse than a rank-one factorization giving a RMSE of 0.91).

$$
\begin{array}{c|cccccccc}
 r & 1 & 5 & 10 & 20 & 50 & 100 \\
 BSSMF & 0.97 \pm 2 \cdot 10^{-5} & 0.87 \pm 0.001 & 0.86 \pm 0.002 & 0.87 \pm 0.002 & 0.88 \pm 0.002 & 0.89 \pm 0.003 \\
 NMF & 0.91 \pm 2 \cdot 10^{-5} & 0.87 \pm 0.003 & 0.87 \pm 0.001 & 0.87 \pm 0.002 & 0.90 \pm 0.004 & 0.92 \pm 0.003 \\
 MF & 0.91 \pm 5 \cdot 10^{-6} & 0.87 \pm 0.003 & 0.87 \pm 0.002 & 0.88 \pm 0.002 & 0.93 \pm 0.004 & 0.99 \pm 0.004 \\
\end{array}
$$

Table 1: RMSE on the testing set according to $r$, averaged ± standard deviation on 10 runs on ml-1m

The same experiment is conducted on the ml-100k dataset which contains 100,000 ratings from 1,700 movies rated by 1,000 users. The testing set contains 50 users. The results are reported in Table 2, and the observations are similar: BSSMF is significantly more robust to overfitting than NMF and unconstrained MF.

$$
\begin{array}{c|cccccccc}
 r & 1 & 5 & 10 & 20 & 50 & 100 \\
 BSSMF & 0.98 \pm 1 \cdot 10^{-4} & 0.89 \pm 0.005 & 0.90 \pm 0.008 & 0.91 \pm 0.01 & 0.93 \pm 0.01 & 0.94 \pm 0.01 \\
 NMF & 0.91 \pm 3 \cdot 10^{-5} & 0.89 \pm 0.01 & 0.90 \pm 0.009 & 0.93 \pm 0.01 & 0.97 \pm 0.01 & 1.01 \pm 0.007 \\
 MF & 0.91 \pm 5 \cdot 10^{-5} & 0.89 \pm 0.008 & 0.92 \pm 0.01 & 0.97 \pm 0.02 & 1.06 \pm 0.03 & 1.13 \pm 0.02 \\
\end{array}
$$

Table 2: RMSE on the testing set according to $r$, averaged ± standard deviation on 10 runs on ml-100k

6 Conclusion

In this paper, we proposed a new factorization model, namely bounded simplex structured matrix factorization (BSSMF). Fitting this model retrieves interpretable factors: the learned basis features can be interpreted in the same way as the original data while the activations are nonnegative and sum to one, leading to a straightforward soft clustering interpretation. Instead of learning parts of objects as NMF, BSSMF learns objects that can be used to explain the data through convex combinations.

We have proposed a dedicated fast algorithm for BSSMF, and showed that, under mild conditions, BSSMF is essentially unique. We also showed that the constraints in BSSMF make it robust to overfitting on rating datasets without adding any regularization term.

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https://grouplens.org/datasets/movielens/100k/
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