Convergence Analysis of Single Latent Factor-dependent, Non-negative and Multiplicative Update-based Non-negative Latent Factor Models

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Abstract—A single latent factor-dependent, non-negative and multiplicative update (SLF-NMU) learning algorithm is highly efficient in building a non-negative latent factor (NLF) model defined on an HiDS matrix. However, convergence characteristics of such NLF models are never justified in theory. To address this issue, this study conducts rigorous convergence analysis for an SLF-NMU-based NLF model. The main idea is two-fold, a) proving that its learning objective keeps non-increasing with its SLF-NMU-based learning rules via constructing specific auxiliary functions, and b) proving that it converges to a stable equilibrium point with its SLF-NMU-based learning rules via analyzing the Karush-Kuhn-Tucker (KKT) conditions of its learning objective. Experimental results on ten HiDS matrices from real applications provide numerical evidence that indicates the correctness of the achieved proof.

Index Terms—Learning System, Single Latent Factor-dependent Non-negative and Multiplicative Update, Non-negative Latent Factor Analysis, Neural Networks, Convergence, Latent Factor Analysis, High-Dimensional and Sparse Matrix, Big Data

I. INTRODUCTION

<u>HIGH-DIMENSIONAL AND SPARSE (HiDS) matrix is</u> commonly adopted to describe incomplete interactions among concerning objects in big data-related applications, e.g., user-service invocations in services computing [1], [3], user-item preferences in recommender systems [4], and protein interactomes in bioinformatics [7]. Despite its extreme sparsity,

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it contains tremendously useful knowledge such as potential links [11]-[13], community tendency [14]-[16], [54] and cluster [17], [35]. A latent factor (LF)-based approach [4], [5], [18], [19] can efficiently implement knowledge acquisition from an HiDS matrix. It works by 1) mapping concerned objects into a low-dimensional LF space, 2) defining a learning objective on the known data of an HiDS target with desired LFs, and 3) optimizing the objective to achieve LFs precisely outlining concerned objects, which are useful in addressing subsequent learning tasks like missing data recovering [9]-[17], [43].

Non-negativity is a common characteristic of most real data, e.g., social impacts from social network services applications [16], [27]. To well represent their non-negativity, an LF model should be restricted to be non-negative [3], [26], [28]. A non-negative matrix factorization (NMF) model [29]-[36], [48]-[52] is designed to address full matrices under the non-negative constraints, but it cannot address an HiDS one directly. Although such a defect can be overcome via specific model designs like weight indication [48] or intermediate matrix incorporation [49], it further suffers high costs in both computation and storage. This is because its costs are proportional to the target matrix's full size [3], [28]. When the target is HiDS, its full size can be much larger than the size of its known data. For instance, the MovieLens 20M [44] matrix's full size is 3.7 billion, while the density of its known data is 0.54%. Due to its extremely low density, it is very inefficient to make a model's costs linear with its full size.

For efficiently implementing non-negative latent factor (NLF) analysis on an HiDS matrix, Luo et al. [3], [28] present a single latent factor-dependent, non-negative and multiplicative update (SLF-NMU) algorithm. It is defined on an HiDS matrix's known data, thereby reducing the storage and computational costs to be linear with the size of its known data. Although it builds an NLF model with high efficiency, its convergence characteristics are never justified formally. For addressing this issue, this paper aims at theoretically proving that an NLF model converges to a Karush-Kuhn-Tucker (KKT) equilibrium point with an SLF-NMU learning algorithm. Main contributions of this work include

- a) Rigorous proof demonstrating that an SLF-NMU-based NLF model's learning objective is non-increasing during the training process via building specific auxiliary functions corresponding to its parameter update rules;
- b) Rigorous proof demonstrating that an SLF-NMU-based NLF model's parameter learning sequence converges to a KKT

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equilibrium point of its learning objective; and

c) Detailed empirical studies on ten HiDS matrices collected by big data-related applications.

Note that convergence analysis for a non-convex learning model is critical in the optimization community [2], [5], [6], [8], [21]-[25]. According to prior research [3], [11], [12], an SLF-NMU-based NLF model is a bi-linear and thus non-convex learning model. Therefore, its rigorous convergence proof is highly useful in providing insights into its learning ability with an HiDS matrix as its input. Moreover, as discussed in [66], [67], performing LF analysis on an HiDS matrix is actually equivalent to building a single-layered neural network whose inputs and outputs are both the target HiDS matrix. Note that in big data-related applications, HiDS matrices are far more frequently encountered than complete ones [3], [68]. It is becoming increasingly important to design a neural network-based learning system with incomplete inputs [3], [66]-[70]. Therefore, results achieved in this study can help people better understand the characteristics of a neural network defined on incomplete data.

The remainder of this paper is organized as follows. Section II gives the preliminaries. Section III presents rigorous proof regarding the convergence of an SLF-NMU-based NLF model. Section IV provides empirical studies. Section V discusses several critical points. Finally, Section VI concludes the paper.

II. PRELIMINARIES

A. Problem Formulation

For LF analysis, we recall the definition of an HiDS matrix [3], [11], [12],

Definition 1. Let *M* and *N* be two large entity sets, $Y^{|M| \times |N|}$ be a matrix whose element $y_{m,n}$ quantifies the interaction between $m \in M$ and $n \in N$, Λ and Γ be *Y*'s known and unknown subsets. *Y* is an HiDS matrix if $|\Lambda| \ll |\Gamma|$.

Based on Λ , an LF model implements a rank-*d* estimation $\hat{Y}=AX^{T}$ for *Y* with $A^{|M|\times d}$ and $X^{|N|\times d}$ being LF matrices. It should be pointed out that *d* is far less than the minimum of |M| and |N|. For achieving *A* and *X*, we construct a loss function to measure the difference between *Y* and \hat{Y} depending on Λ only. Based on the Euclidean distance, it is given by

$$\varepsilon(A,X) = \frac{1}{2} \sum_{y_{m,n} \in \Lambda} \left(y_{m,n} - \sum_{k=1}^{d} a_{m,k} x_{n,k} \right)^2, \qquad (1)$$

where $a_{m,k}$, $x_{n,k}$ and $y_{m,n}$ denote specified elements in A, X, and Y. For correctly representing non-negative data [1], [3], [11]-[13], [16], [19], [27], (1) should fulfill the non-negativity constraints,

$$a_{m,k} \ge 0, x_{n,k} \ge 0, \forall m \in M, n \in N, k \in \{1, 2, ..., d\}.$$
 (2)

Meanwhile, building an LF model on an HiDS matrix is ill-posed [3], [28], [42], making regularizations indispensable. Let $\hat{y}_{m,n} = \sum_{k=1}^{d} a_{m,k} x_{n,k}$, we reformulate (2) to incorporate L_2 norm-based regularizations into it,

$$\varepsilon(A,X) = \frac{1}{2} \sum_{y_{m,n} \in \Lambda} \left(\left(y_{m,n} - \hat{y}_{m,n} \right)^2 + \lambda_A \sum_{k=1}^d a_{m,k}^2 + \lambda_X \sum_{k=1}^d x_{n,k}^2 \right),$$
(3)
s.t. $a_{m,k} \ge 0, x_{n,k} \ge 0, \forall m \in M, n \in N, k \in \{1, 2, ..., d\}.$

where λ_A and λ_X denote the regularization constants for *A* and *X*, respectively.

B. A Non-negative Latent Factor Model

An NLF model adopts an SLF-NMU-based learning algorithm to optimize A and X in (3). It initially applies additive gradient descent (AGD) to each LF:

$$\arg\min_{A,X} \varepsilon(A,X) \stackrel{AGD}{\Rightarrow} \begin{cases} a_{m,k} \leftarrow a_{m,k} - \eta_{m,k} \sum_{n \in \Lambda(m)} (\lambda_A a_{m,k} - x_{n,k} (y_{m,n} - \hat{y}_{m,n})), \\ x_{n,k} \leftarrow x_{n,k} - \eta_{n,k} \sum_{m \in \Lambda(n)} (\lambda_X x_{n,k} - a_{m,k} (y_{m,n} - \hat{y}_{m,n})). \end{cases}$$
(4)

where $\eta_{m,k}$ and $\eta_{n,k}$ are learning rates for $a_{m,k}$ and $x_{n,k}$, $\Lambda(m)$ and $\Lambda(n)$ are Λ 's subsets related to m and n, respectively. From (4), we see that $a_{m,k}$ and $x_{n,k}$ can become negative due to $-\eta_{m,k} \sum_{n \in \Lambda(m)} (x_{n,k} \hat{y}_{m,n} + \lambda_A a_{m,k})$ and $-\eta_{n,k} \sum_{m \in \Lambda(n)} (a_{m,k} \hat{y}_{m,n} + \lambda_X x_{n,k})$.

For canceling these negative terms to keep the non-negativity of *A* and *X*, an SLF-NMU algorithm manipulates $\eta_{m,k}$ and $\eta_{n,k}$,

$$\eta_{m,k} = \frac{u_{m,k}}{\sum_{n \in \Lambda(m)} x_{n,k} \hat{y}_{m,n} + \lambda_A |\Lambda(m)| a_{m,k}},$$

$$\eta_{n,k} = \frac{x_{n,k}}{\sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n} + \lambda_X |\Lambda(n)| x_{n,k}}.$$
(5)

By combining (5) and (4), we achieve the learning rules for an SLF-NMU-based NLF model [28]:

$$\arg\min_{A,X} \mathcal{E}\left(A,X\right) \stackrel{\text{SLF-INAC}}{\Rightarrow} \left\{ \begin{aligned} a_{m,k} \leftarrow a_{m,k} \frac{\sum_{n \in \Lambda(m)} x_{n,k} y_{m,n}}{\sum_{n \in \Lambda(m)} x_{n,k} \hat{y}_{m,n} + \lambda_A \left| \Lambda(m) \right| a_{m,k}}, \\ x_{n,k} \leftarrow x_{n,k} \frac{\sum_{m \in \Lambda(n)} a_{m,k} y_{m,n}}{\sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n} + \lambda_X \left| \Lambda(n) \right| x_{n,k}}. \end{aligned} \right.$$

C. Incorporation of Linear Biases

As discussed in previous studies [20], [22], incorporating linear biases makes an NLF model become more steadily during the training process, at the same time obtain higher accuracy for estimating missing entries of a target HiDS matrix. With linear bias vectors $B^{[M]}$ and $C^{[N]}$ for M and N, respectively, the objective function (3) is reformulated into

$$\begin{split} \varepsilon(A, X, B, C) &= \\ \frac{1}{2} \sum_{y_{m,n} \in \Lambda} \left(\left(y_{m,n} - \hat{y}_{m,n} \right)^2 + \lambda_A \sum_{k=1}^d a_{m,k}^2 + \lambda_X \sum_{k=1}^d x_{n,k}^2 + \lambda_B b_m^2 + \lambda_C c_n^2 \right), \\ s.t. \quad a_{m,k} \ge 0, x_{n,k} \ge 0, b_m \ge 0, c_n \ge 0, \\ \forall m \in M, n \in N, k \in \{1, 2, \dots, d\}, \end{split}$$
(7)

where each approximation $\hat{y}_{m,n}$ to $y_{m,n} \in \Lambda$ is given by

$$\hat{y}_{m,n} = \sum_{k=1}^{d} a_{m,k} x_{n,k} + b_m + c_n.$$
(8)

Following the same principle of (6), we have the learning rules for a biased NLF (BNLF) model,

$$\operatorname{arg min}_{A,X,B,C} \varepsilon \left(A,X,B,C\right)^{SLF-NMU} \Rightarrow
 \left\{ b_{m} \leftarrow b_{m} \sum_{n \in \Lambda(m)} y_{m,n} \middle/ \left(\sum_{n \in \Lambda(m)} \hat{y}_{m,n} + \lambda_{B} \middle| \Lambda(m) \middle| b_{m} \right), \\ c_{n} \leftarrow c_{n} \sum_{m \in \Lambda(n)} y_{m,n} \middle/ \left(\sum_{m \in \Lambda(n)} \hat{y}_{m,n} + \lambda_{C} \middle| \Lambda(n) \middle| c_{n} \right), \\ a_{m,k} \leftarrow a_{m,k} \sum_{n \in \Lambda(m)} x_{n,k} y_{m,n} \middle/ \left(\sum_{n \in \Lambda(m)} x_{n,k} \hat{y}_{m,n} + \lambda_{A} \middle| \Lambda(m) \middle| a_{m,k} \right), \\ x_{n,k} \leftarrow x_{n,k} \sum_{m \in \Lambda(n)} a_{m,k} y_{m,n} \middle/ \left(\sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n} + \lambda_{X} \middle| \Lambda(n) \middle| x_{n,k} \right).$$
(9)

III. CONVERGENCE ANALYSIS OF THE NON-NEGATIVE LATENT FACTOR MODEL

A. An Alternative Way to Achieve an SLF-NMU Algorithm

It is firstly necessary to discover the connections between an SLF-NMU algorithm and the KKT conditions [46], [52], [54] of the learning objective (6). Let $K=[\kappa_{m,k}]$, $\Phi=[\phi_{n,k}]$ be Lagrangian multipliers for the non-negative constraints $a_{m,k}\ge 0$ and $x_{n,k}\ge 0$, respectively. Then the Lagrangian *L* for (3) is:

$$L = \varepsilon(A, X) - Tr(\mathbf{K}A^{\mathrm{T}}) - Tr(\mathbf{\Phi}X^{\mathrm{T}})$$
$$= \varepsilon(A, X) - \sum_{m=1}^{|M|} \sum_{k=1}^{d} \kappa_{m,k} a_{m,k} - \sum_{n=1}^{|N|} \sum_{k=1}^{d} \phi_{n,k} x_{n,k}, \qquad (10)$$

where $Tr(\cdot)$ calculates the trace of an enclosed matrix. Considering the partial derivatives of *L* with $a_{m,k}$ and $x_{n,k}$:

$$\begin{cases} \frac{\partial L}{\partial a_{m,k}} = \sum_{n \in \Lambda(m)} \left(\lambda_A a_{m,k} - x_{n,k} \left(y_{m,n} - \hat{y}_{m,n} \right) \right) - \kappa_{m,k} = 0, \\ \frac{\partial L}{\partial x_{n,k}} = \sum_{m \in \Lambda(n)} \left(\lambda_X x_{n,k} - a_{m,k} \left(y_{m,n} - \hat{y}_{m,n} \right) \right) - \phi_{n,k} = 0; \\ \end{cases}$$

$$\Rightarrow \begin{cases} \kappa_{m,k} = \sum_{n \in \Lambda(m)} \left(\lambda_A a_{m,k} - x_{n,k} \left(y_{m,n} - \hat{y}_{m,n} \right) \right), \\ \phi_{n,k} = \sum_{m \in \Lambda(n)} \left(\lambda_X x_{n,k} - a_{m,k} \left(y_{m,n} - \hat{y}_{m,n} \right) \right). \end{cases}$$

$$(11)$$

Then considering the KKT conditions of (10), i.e., $\kappa_{m,k}a_{m,k}=0$, $\forall \kappa_{m,k}, a_{m,k}$, and $\phi_{n,k}x_{n,k}=0$, $\forall \phi_{n,k}, x_{n,k}$, we achieve that

$$\begin{cases} a_{m,k} \sum_{n \in \Lambda(m)} \left(\lambda_{A} a_{m,k} - x_{n,k} \left(y_{m,n} - \hat{y}_{m,n} \right) \right) = 0, \\ x_{n,k} \sum_{m \in \Lambda(n)} \left(\lambda_{X} x_{n,k} - a_{m,k} \left(y_{m,n} - \hat{y}_{m,n} \right) \right) = 0. \end{cases}$$
(12)

With (12), we arrive at the following iterative equations which actually lead to (6),

$$\begin{cases} a_{m,k} \sum_{n \in \Lambda(m)} x_{n,k} y_{m,n} = a_{m,k} \left(\lambda_A \left| \Lambda(m) \right| a_{m,k} + \sum_{n \in \Lambda(m)} x_{n,k} \hat{y}_{m,n} \right), \\ x_{n,k} \sum_{m \in \Lambda(n)} a_{m,k} y_{m,n} = x_{n,k} \left(\lambda_X \left| \Lambda(n) \right| x_{n,k} + \sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n} \right); \\ \Rightarrow \begin{cases} a_{m,k} \leftarrow a_{m,k} \frac{\sum_{n \in \Lambda(m)} x_{n,k} y_{m,n}}{\lambda_A \left| \Lambda(m) \right| a_{m,k} + \sum_{n \in \Lambda(m)} x_{n,k} \hat{y}_{m,n}}, \\ x_{n,k} \leftarrow x_{n,k} \frac{\sum_{m \in \Lambda(n)} a_{m,k} y_{m,n}}{\lambda_X \left| \Lambda(n) \right| x_{n,k} + \sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n}}. \end{cases}$$
(13)

From (10)-(13), we see that the SLF-NMU-based learning rules in an NLF model are closely connected to the KKT conditions of its learning objective.

B. Convergence Analysis of an NLF model

In this part, we theoretically analyze the convergence of an SLF-NMU learning algorithm in the following two steps. *1) Non-increasing learning objective with SLF-NMU.*

In this step, we aim to prove that (3) is non-increasing with (6). To do so, we have

Theorem 1. (3) is non-increasing with (6).

To prove Theorem 1, an auxiliary function [31], [53] is vital.

Definition 2. G(x, x') is an auxiliary function of F(x) if

$$G(x,x') \ge F(x), \ G(x,x) = F(x). \tag{14}$$

We further recall the following lemma [31], [53],

Lemma 1. F keeps non-increasing with the following rule,

$$x^{t+1} = \arg\min_{x} G(x, x^t).$$
(15)

Proof of Lemma 1. With Definition 2, we deduce that

$$F\left(x^{t}\right) = G\left(x^{t}, x^{t}\right) \ge G\left(x^{t+1}, x^{t}\right) \ge F\left(x^{t+1}\right).$$
(16)

Note that we have $F(x^{t+1})=F(x^t)$ when x^t guarantees a local minimum of $G(x, x^t)$, Hence, $\nabla F(x^t)=0$ holds if F is differentiable around x^t . Hence, (16) can be extended into the following converging sequence to $x_{\min}=\arg \min_x F(x)$,

$$F(x_{\min}) \leq \cdots \leq F(x^{t+1}) \leq F(x^{t}) \leq \cdots \leq F(x_{1}) \leq F(x_{0}).$$
(17)

Next, we aim to achieve that (6) for is exactly consistent with that in (15) with a specifically designed *G*. Considering $x_{n,k} \in X$, let $F_{x_{n,k}}$ be the partial loss from $\varepsilon(A, X)$ related to $x_{n,k}$ only,

$$F_{x_{n,k}} = \frac{1}{2} \sum_{y_{m,n} \in \Lambda} \left(\left(y_{m,n} - \hat{y}_{m,n} \right)^2 + \lambda_A \sum_{k=1}^d a_{m,k}^2 + \lambda_X \sum_{k=1}^d x_{n,k}^2 \right), \quad (18)$$

where $\hat{y}_{m,n} = a_{m,k} x_{n,k} + \sum_{l=1, \neq k}^d a_{m,l} x_{n,l}$.

So we have the first-order and second-order derivatives of $F_{x_{n,k}}$ with respect to $x_{n,k}$,

$$F_{x_{n,k}}' = \frac{\partial \varepsilon}{\partial x_{n,k}} = \lambda_X \left| \Lambda(n) \right| x_{n,k} + \sum_{m \in \Lambda(n)} \left(-a_{m,k} \left(y_{m,n} - \hat{y}_{m,n} \right) \right), \quad (19)$$

$$F_{x_{n,k}}'' = \frac{\partial^2 \varepsilon}{\partial (x_{n,k})^2} = \lambda_X \left| \Lambda(n) \right| + \sum_{m \in \Lambda(n)} (a_{m,k})^2.$$
(20)

Based on (18)-(20), we achieve the following proposition. *Proposition* **1.** The following function

$$G\left(x, x_{n,k}^{(t)}\right) = F_{x_{n,k}}\left(x_{n,k}^{(t)}\right) + F'_{x_{n,k}}\left(x_{n,k}^{(t)}\right) \left(x - x_{n,k}^{(t)}\right) + \frac{1}{2} \left(\lambda_{x} \left|\Lambda\left(n\right)\right| x_{n,k}^{(t)} / x_{n,k}^{(t)} + \sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n}\right) \left(x - x_{n,k}^{(t)}\right)^{2}$$
(21)

is an auxiliary function of $F_{x_{n,k}}$.

Proof of Proposition 1. With (21), $G(x,x) = F_{x_{n,k}}(x)$ holds. Then we aim to prove $G(x, x_{n,k}^{(t)}) \ge F_{x_{n,k}}(x)$. To do so, we first derive the quadratic approximation to $F_{x_{n,k}}$ at $x_{n,k}^{(t)}$.

$$F_{x_{n,k}}(x) = F_{x_{n,k}}(x_{n,k}^{(t)}) + F_{x_{n,k}}'(x_{n,k}^{(t)})(x - x_{n,k}^{(t)}) + \frac{1}{2}F_{x_{n,k}}''(x_{n,k}^{(t)})(x - x_{n,k}^{(t)})^{2}.$$
(22)

By combining (20-22), we see that $G(x, x_{n,k}^{(t)})$ is an auxiliary function of $F_{x_{n,k}}$ if the following inequality holds,

$$\frac{\lambda_{X} \left| \Lambda(n) \right| x_{n,k}^{(t)} + \sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n}}{x_{n,k}^{(t)}} \geq \lambda_{X} \left| \Lambda(n) \right| + \sum_{m \in \Lambda(n)} \left(a_{m,k} \right)^{2}.$$
(23)

Note that we have $y_{m,n} \ge 0$ according to *Y*'s non-negativity, and $a_{m,k} \ge 0$, and $x_{n,k} \ge 0$ with SLF-NMU. So (23) is equal to

$$\sum_{m\in\Lambda(n)} a_{m,k} \hat{y}_{m,n} \ge x_{n,k}^{(t)} \sum_{m\in\Lambda(n)} \left(a_{m,k}\right)^2.$$
(24)

Then we reformulate the left term of (24) as follows:

$$\sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n} = \sum_{m \in \Lambda(n)} a_{m,k} \left[a_{m,k} x_{n,k}^{(t)} + \sum_{l=1,l \neq k}^{\infty} a_{m,l} x_{n,l} \right]$$

= $x_{n,k}^{(t)} \sum_{m \in \Lambda(n)} (a_{m,k})^2 + \sum_{m \in \Lambda(n)} \left[a_{m,k} \sum_{l=1,l \neq k}^{d} a_{m,l} x_{n,l} \right]$ (25)
 $\geq x_{n,k}^{(t)} \sum_{m \in \Lambda(n)} (a_{m,k})^2.$

Note that (23) holds with (25), making $G(x, x_{n,k}^{(t)})$ be an auxiliary function of $F_{x_{n,k}}$.

Based on Proposition 1, we achieve the following proof. **Proof of Theorem 1.** Based on (15), (19) and (21), we achieve $x_{n\,k}^{(t+1)} = \arg\min G(x, x_{n,k}^{(t)})$

$$\Rightarrow F'_{x_{n,k}}\left(x_{n,k}^{(t)}\right) + \frac{\sum_{m \in \Lambda(n)}^{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n} + \lambda_X \left|\Lambda(n)\right| x_{n,k}^{(t)}}{x_{n,k}^{(t)}} \left(x - x_{n,k}^{(t)}\right) = 0 (26)$$

$$\Rightarrow x_{n,k}^{(t+1)} \leftarrow x_{n,k}^{(t)} \frac{\sum_{m \in \Lambda(n)}^{m \in \Lambda(n)} a_{m,k} y_{m,n}}{\sum_{m \in \Lambda(n)}^{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n} + \lambda_X \left|\Lambda(n)\right| x_{n,k}^{(t)}}.$$

Based on (26), it is clear that $F_{x_{n,k}}$ is non-increasing with (6).

Naturally, (26) holds $\forall n \in N, m \in M, k \in \{1, 2, ..., d\}$. Hence, Theorem 1 holds.

Following Theorem 1, with a positive initialization, i.e., $\forall m \in M, n \in N$ and $k \in \{1, 2, ..., d\}$: $a_{m,k}^{(0)}$, $x_{n,k}^{(0)} > 0$, (3) is non-increasing when training A and X with (6). From this point of view, we have the following recursion,

$$F\left(x_{n,k}^{(0)}\right) \ge F\left(x_{n,k}^{(t)}\right) \ge G\left(x_{n,k}^{(t+1)}, x_{n,k}^{(t)}\right) \ge F\left(x_{n,k}^{(t+1)}\right) \ge 0, \quad (27)$$

which indicates that a sequence $\{F(x_{n,k}^{(t)})\}$ is monotonically non-increasing and bounded. Hence, we deduce that

$$\lim_{t \to +\infty} \left(F\left(x_{n,k}^{(t+1)}\right) - F\left(x_{n,k}^{(t)}\right) \right) = 0.$$
(28)

With (28), we further have the following inference,

$$\lim_{t \to +\infty} \left| x_{n,k}^{(t+1)} - x_{n,k}^{(t)} \right| = 0.$$
⁽²⁹⁾

Therefore, a sequence $\{x_{n,k}^{(t)}\}$ is bounded and convergent. Similarly, a sequence $\{a_{m,k}^{(t)}\}$ is also bounded and convergent. 2) Sequences $\{a_{m,k}^{(t)}\}$ and $\{x_{n,k}^{(t)}\}$ by SLF-NMU converge to a KKT equilibrium point of (3). To prove it, we have

Theorem 2. Sequences $\{a_{m,k}^{(t)}\}$ and $\{x_{n,k}^{(t)}\}$ by (6) converge to an equilibrium point $(a_{m,k}^{(*)}, x_{n,k}^{(*)})$ of $\varepsilon(A, X)$ in (3).

Proof of Theorem 2. Based on (29), a sequence $\{x_{n,k}^{(t)}\}$ converges with (6). Let $X^{(*)}$ denote a stationary point of X, i.e., $0 \le x_{n,k}^{(*)} = \lim_{t \to +\infty} x_{n,k}^{(t)} < +\infty$, $\forall n \in N$, $k \in \{1, 2, ..., d\}$. Thus, the following KKT conditions of (3) regarding X should be satisfied, if $X^{(*)}$ is one of its equilibrium points.

 $\forall n \in N, m \in M, k \in \{1, \dots, d\}$:

(a)
$$\frac{\partial L}{\partial x_{n,k}}\Big|_{x_{n,k}=x_{n,k}^{(*)}} = \sum_{m\in\Lambda(n)} \left(\lambda_X x_{n,k}^{(*)} - a_{m,k} \left(y_{m,n} - \hat{y}_{m,n}\right)\right) - \phi_{n,k}^{(*)} = 0,$$

(b) $\phi_{n,k}^{(*)} \cdot x_{n,k}^{(*)} = 0,$
(c) $x_{n,k}^{(*)} \ge 0,$
(d) $\phi_{n,k}^{(*)} \ge 0.$
(30)

Note that following (10)-(13), Condition (a) is naturally fulfilled with (6) and (13). Thus, we actually have

$$\phi_{n,k}^{(*)} = \sum_{m \in \Lambda(n)} \left(\lambda_X x_{n,k}^{(*)} - a_{m,k} \left(y_{m,n} - \hat{y}_{m,n} \right) \right).$$
(31)

Thus, we focus on Conditions (c)-(d). We start with constructing $\theta_{n,k}^{(t)}$,

$$\theta_{n,k}^{(t)} = \frac{\sum_{m \in \Lambda(n)} a_{m,k} y_{m,n}}{\lambda_X \left| \Lambda(n) \right| x_{n,k}^{(t)} + \sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n}}.$$
(32)

Obviously, (32) is bounded by non-negative $a_{m,k}$ and $y_{m,n}$:

$$0 \le \theta_{n,k}^{(*)} = \lim_{t \to +\infty} \theta_{n,k}^{(t)} = \frac{\sum_{m \in \Lambda(n)} a_{m,k} y_{m,n}}{\lambda_X \left| \Lambda(n) \right| x_{n,k}^{(*)} + \sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n}}.$$
 (33)

Hence, the update rule of $x_{n,k}$ can be rewritten with SLF-NMU, $x_{n,k}^{(t+1)} = x_{n,k}^{(t)} \theta_{n,k}^{(t)}.$ (34)

By combining (29) and (34), we have

$$\lim_{t \to \infty} \left| x_{n,k}^{(t+1)} - x_{n,k}^{(t)} \right| = 0 \Longrightarrow x_{n,k}^{(*)} \theta_{n,k}^{(*)} - x_{n,k}^{(*)} = 0.$$
(35)

Note that following the update rule (13), $x_{n,k}^{(*)}$ is greater than or equal to zero with a non-negatively initial hypothesis. Hence, we have the following inferences.

a) When $x_{n,k}^{(*)} > 0$. Based on (32) and (35), we have:

$$\begin{aligned} x_{n,k}^{(*)} \theta_{n,k}^{(*)} - x_{n,k}^{(*)} &= 0, \\ x_{n,k}^{(*)} > 0 \Longrightarrow \theta_{n,k}^{(*)} &= 1 \\ \Longrightarrow \lambda_{\chi} \left| \Lambda(n) \right| x_{n,k}^{(*)} + \sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n} - \sum_{m \in \Lambda(n)} a_{m,k} y_{m,n} &= 0. \end{aligned}$$
(36)

Combining (31) and (36), we obtain the Condition (b) in (30),

$$\phi_{n,k}^{(*)} = \lambda_X \left| \Lambda(n) \right| x_{n,k}^{(*)} + \sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n} - \sum_{m \in \Lambda(n)} a_{m,k} y_{m,n} = 0
\Rightarrow \phi_{n,k}^{(*)} \cdot x_{n,k}^{(*)} = 0.$$
(37)

Meanwhile, when $\phi_{n,k}^{(*)} = 0$ and $x_{n,k}^{(*)} > 0$, Conditions (c) and (d) are naturally fulfilled. Hence, (30) is fulfilled when $x_{n,k}^{(*)} > 0$.

b) When $x_{n,k}^{(*)} = 0$. Note that conditions (b) and (c) in (30) are naturally fulfilled in this case. Hence, we want to justify Condition (d). To do so, we reformulate $x_{n,k}^{(*)}$ into

$$\mathbf{x}_{n,k}^{(*)} = \mathbf{x}_{n,k}^{(0)} \lim_{t \to +\infty} \prod_{r=1}^{l} \boldsymbol{\theta}_{n,k}^{(r)}.$$
 (38)

Based on (38) we further have the following inferences,

$$x_{n,k}^{(0)} > 0, x_{n,k}^{(0)} \lim_{t \to +\infty} \prod_{r=1}^{t} \theta_{n,k}^{(r)} = x_{n,k}^{(*)} = 0 \Longrightarrow \lim_{t \to +\infty} \prod_{r=1}^{t} \theta_{n,k}^{(r)} = 0$$
$$\Rightarrow \lim_{t \to +\infty} \theta_{n,k}^{(t)} = \theta_{n,k}^{(*)} = \frac{\sum_{m \in \Lambda(n)} a_{m,k} y_{m,n}}{\lambda_X |\Lambda(n)| x_{n,k}^{(*)} + \sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n}} \le 1$$
(39)

$$\Rightarrow \phi_{n,k}^{(*)} = \lambda_X \left| \Lambda(n) \right| x_{n,k}^{(*)} + \sum_{m \in \Lambda(n)} a_{m,k} \hat{y}_{m,n} - \sum_{m \in \Lambda(n)} a_{m,k} y_{m,n} \ge 0.$$

Hence, (30) is also fulfilled when $x_{n,k}^{(*)} > 0$. Analogously, we can prove that sequence $\{a_{m,k}^{(t)}\}$ also converges to an stable equilibrium point of (3). Thus, Theorem 2 stands.

By combining Theorems 1 and 2, we have proven that an SLF-NMU-based NLF model converges to a KKT equilibrium point of its objective. It should be pointed out a positive initialization of LFs is helpful in achieving an optimal solution, which is consistent with [55].

C. Convergence Analysis of a BNLF model

1) Non-increasing learning objective with biased SLF-NMU. We firstly present the following theorem.

Theorem 3. (7) is non-increasing with (9).

Note that for Theorem 3, we only have to analyze the partial

loss with *B* and *C* since conditions of *A* and *X* are highly similar with that in an NLF model as shown in Theorem 1. Considering $b_m \in B$, let \tilde{F}_{b_m} be the partial loss of $\varepsilon(A, X, B, C)$ related to b_m only. Then we derive the first-order and second-order derivatives of \tilde{F}_{b_m} with respect to b_m ,

$$\tilde{F}_{b_m}' = \lambda_B \left| \Lambda(m) \right| b_m - \sum_{n \in \Lambda(m)} \left(y_{m,n} - \hat{y}_{m,n} \right).$$
(40)

$$\tilde{F}_{b_m}'' = (1 + \lambda_\beta) |\Lambda(m)|.$$
(41)

Based on (7), (40) and (41), we present Proposition 2. **Proposition 2.** The following function

$$\tilde{G}(b, b_{m}^{(t)}) = \tilde{F}_{b_{m}}(b_{m}^{(t)}) + \tilde{F}_{b_{m}}'(b_{m}^{(t)})(b - b_{m}^{(t)}) + \frac{1}{2} \left(\sum_{n \in \Lambda(m)} (\hat{y}_{m,n} + \lambda_{B} b_{m}^{(t)}) / b_{m}^{(t)} \right) (b - b_{m}^{(t)})^{2},$$
(42)

is an auxiliary function of \tilde{F}_{b_m} .

Note that the proof of Proposition 2 is provided in the supplementary file of this paper. With it we prove Theorem 3, whose proof is also provided in the supplementary file.

Following Theorems 1 and 3, with a positive initialization, i.e., $\forall m \in M$, $n \in N$, and $k \in \{1, 2, ..., d\}$: $a_{m,k}^{(0)}$, $x_{n,k}^{(0)}$, $b_m^{(0)}$ and $c_n^{(0)} > 0$, (7) is non-increasing when training *A*, *X*, *B* and *C* with (9). From this point of view, we have the following recursion:

$$\tilde{F}\left(b_{m}^{(0)}\right) \geq \tilde{F}\left(b_{m}^{(t)}\right) \geq \tilde{G}\left(b_{m}^{(t+1)}, b_{m}^{(t)}\right) \geq \tilde{F}\left(b_{m}^{(t+1)}\right) \geq 0, \quad (43)$$

which indicates that a sequence $\left\{\tilde{F}\left(b_{m}^{(t)}\right)\right\}$ is non-increasing and bounded. Hence, we deduce that

$$\lim_{t \to +\infty} \left| \tilde{F} \left(b_m^{(t+1)} \right) - \tilde{F} \left(b_m^{(t)} \right) \right| = 0.$$
(44)

Based on (49), we further yield the following inference:

$$\lim_{t \to +\infty} \left| b_m^{(t+1)} - b_m^{(t)} \right| = 0.$$
 (45)

Therefore, a sequence $\{b_n^{(t)}\}\$ is convergent and bounded. Similarly, a sequence $\{c_n^{(t)}\}\$ is also convergent and bounded.

2) Sequences $\{a_{m,k}^{(t)}\}$, $\{x_{n,k}^{(t)}\}$, $\{b_m^{(t)}\}$ and $\{c_n^{(t)}\}$ by a biased SLF-NMU converge to a KKT equilibrium point of (7).

To prove it, we have the following theorem.

Theorem 4. Sequences $\{a_{m,k}^{(t)}\}$, $\{x_{n,k}^{(t)}\}$, $\{b_m^{(t)}\}$ and $\{c_n^{(t)}\}$ by (9) converge to an equilibrium point of (7).

Note that its proof is provided in the supplementary file. By analogy, we prove that sequence $\{c_n^{(i)}\}$ also converges to an equilibrium point of (7).

Hence, by combining Theorems 1-4, we arrive at the conclusion that a BNLF model converges to a KKT equilibrium point of its objective with a biased SLF-NMU algorithm.

IV. EXPERIMENTAL RESULTS AND ANALYSIS

A. General Settings

Evaluation Metrics. Considering the need for recovering

full links among involved entities [1]-[12] when addressing an HiDS matrix in real applications, the main purpose is to estimate its missing entries. Hence, we adopt the root mean squared error (RMSE) as an evaluation metric to test the reconstruction ability of tested models on an HiDS matrix [3], [11], [12], [28], [47],

$$\text{RMSE} = \sqrt{\frac{1}{|\Psi|} \left(\sum_{r_{u,v} \in T} \left(r_{u,v} - \hat{r}_{u,v} \right)^2 \right)}, \quad (46)$$

where $|\cdot|$ calculates a set's cardinality, Ψ denotes the validation set that is disjoint with the given set Λ , and $\hat{r}_{u,v}$ stands for an estimation for $r_{u,v} \in \Psi$ by a tested model, respectively.

Thus, the convergence behaviors of a tested model are reflected by three factors, i.e., a) its training RMSE, b) its absolute reduction of the learning objective (2), and c) its LF distributions during/after the learning process. All factors are expected to be stable when a model converges. All empirical tests are conducted on a server with a 2.7 GHz E5-2680 V4 CPU and 256 GB RAM, and all models are implemented in JAVA SE 8U131.

Tested Models. As shown in Table I, three models, i.e., NLF [3], BNLF [28], and WNMF [48] are tested and compared.

TABLE I						
	TESTED MODELS IN OUR EXPERIMENTS					
No.	Name	Description				
M1	NLF	Original NLF model relying on the SLF-NMU algorithm proposed in [28].				
M2	BNLF	Biased NLF model by SLF-NMU proposed in [3].				
M3	WNMF	A weighted NMF model proposed in [48]. It can address an HiDS matrix.				

TABLE II DETAILS OF EXPERIMENTAL DATASETS						
No.	Name	$ \Lambda + \Psi $	<i>M</i>	N	Source	
D1	ML20M	20,000,263	138,493	26,744	MovieLens [44]	
D2	NetFlix	100,480,507	2,649,429	17,770	NetFlix [45]	
D3	Douban	16,830,839	129, 490	58, 541	Douban [56]	
D4	Flixter	8,196,077	147,612	48,794	Flixter [61]	
D5	Epinion	13,668,320	120,492	755,760	Truslet website [62]	
D6	Dating	17,359,346	135,359	168,791	LibimSeTi [63]	
D7	EM	2,811,718	72,916	1,628	EachMovie	
D8	Network	175,180	134,007	134,007	Authors' affiliation	
D9	PICE	5,778,268	15,752	15,752	STRING [64]	
D10	PIPA	1.559.616	5,565	5,565	STRING [64]	

Datasets. As recorded in Table II, ten real HiDS matrices collected from industrial applications are adopted. We employ the following settings for objective results.

- a) Each dataset is divided into five disjoint and equally-sized subsets randomly. We adopt the 80%-20% given-validation settings and five-fold cross-validations in all the experiments, i.e., each time we choose four subsets as the given set Λ to build a model to predict missing data and the remaining one as the validation set Ψ to achieve its validation RMSE. Then we sequentially repeat this process five times to conduct five-fold cross-validation for the final results.
- b) When building a model, the given set Λ is further split into two disjoint training and testing subsets with the ratio of 90%: 10%. The model is trained on the training set and tested on the testing set to determine if its training process should be terminated. The training of a model ends if it converges, i.e., its error difference between two successive epochs is less than 10⁻⁵, or its iteration count exceeds a preset threshold, i.e.,

1000.

- c) Making $\lambda_A = \lambda_X = \lambda_B = \lambda_C = \lambda$ for M1-2 following [3], [28], [47] (it should be pointed out that tuning them separately can slightly improve the accuracy of M1-2 but is very time-consuming).
- d) Note that according to [3]-[5], [7]-[12], [28], [47], an NLF model's performance can be affected by its initial hypothesis. Hence, on each testing case, we initialize M1-3 with the same randomly-generated and non-negative arrays for eliminating the influence of an initial hypothesis.

By doing so, we make all involved models built on the given set Λ only. For M1-2, the hyper-parameter λ is tuned on Λ . For M1-3, the training termination is guaranteed on Λ . Each model's reconstruction ability is validated on Ψ separately, whose information is never referred by its training process.

B. Impact of λ

As discussed in prior studies [28], [47], M1-2's performance can be improved significantly via incorporating the Tikhonov regularization. Note that the hyper-parameter λ actually controls the regularization effects in their objective function. They may suffer overfitting as λ becomes too small and underfitting as λ becomes too large. These phenomena are connected with the convergence behaviors of M1-2 and should be carefully validated. We have set λ in the scale of [0.01, 0.20] for demonstrating the former, and set λ =10, 100, and 1000 for demonstrating the latter.

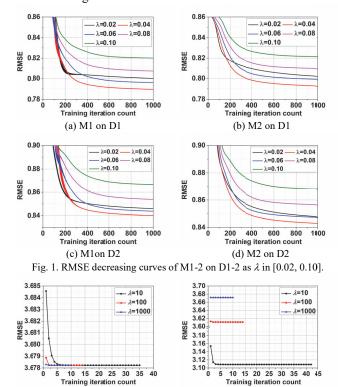


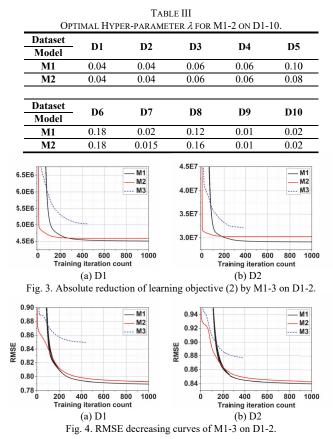
Fig. 2. RMSE decreasing curves of M1-2 on D1 as λ =10, 100, 1000. Fig. 1 depicts the RMSE decreasing curves for M1-2 on D1-2 as λ in [0.02, 0.10]. Fig. 3 depicts the RMSE decreasing curves for M1-2 on D1 as λ =10, 100 and 1000. Similar phenomena are also encountered on D3-10. Moreover, the optimal λ for M1-2

(b) M2

(a) M1

on D1-10 are summarized in Table III. Note that these results are achieved on Λ of D1-10 only, following the settings mentioned in Section IV(A). From them, we find that:

- a) M1-2 suffers overfitting as λ becomes too small, which is reflected by their accuracy loss. From Figs. 1-2, we see that M1-2's RMSE as λ =0.02 is obviously higher than that achieved as λ =0.04. More specifically, M1's RMSE is 0.8001 when λ =0.02, and 0.7895 when λ =0.04. Thus, inappropriately small λ makes it suffer an accuracy loss at 1.34%. Considering M2, its RMSE is 0.8021 as λ =0.02 and 0.7924 as λ =0.04. It turns out that too small λ makes it suffer overfitting, leading to an accuracy loss at 1.20%.
- b) M1-2 suffer underfitting as λ becomes too large, which is also reflected by their accuracy loss. When λ increases over 0.04, M1-2 suffer accuracy loss on D1-2, as shown in Figs. 1-2, which is caused by underfitting. From Fig. 2, we clearly see that as λ increases to 10-1000, M1-2 can still guarantee the convergence to a stable equilibrium point of the objective function. However, they converge to mostly minimize the regularization terms instead of minimizing the generalized error to fit the training data, thereby suffering significant accuracy loss. For example, as depicted in Fig. 2(b), M2's RMSE at 3.6714 when λ =1000, which is about 4.65 times that of 0.7895 when λ =0.04.



C. Convergence Behaviors

In this part of the experiments, we validate the convergence behaviors of M1-2. In addition, we include M3 for comparison. On Λ , each tested model is expected to stabilize its a) Training RMSE, b) absolute reduction of learning objective (2), and c)

LF distribution.

Fig. 3 depicts the absolute reduction of learning objective (2) by M1-3 on D1-2. The RMSE decreasing curves of M1-3 on D1-2 are depicted in Fig. 4. Figs. S1-2 in the Supplementary File of this paper depict LF distributions of M1-2 after the initialization, 1st, 10th, 50th, 100th, 200th, 400th, 600th, 800th, and last iteration during the training process on D1. Note that we present these results only for a concise report. However, highly similar phenomena are encountered in other testing cases. From these results, we have the following findings:

- a) M1-2 converge better than M3 does on an HiDS matrix. From Figs. 3-4, we see that M3 cannot reach a good local optimum, and commonly ends with fewer iterations and higher RMSE when compared with M1-2. For instance, according to Fig. 4(a), on D1 it consumes 441 iterations to obtain the RMSE at 0.8489. In comparison, M1 consumes 1000 iterations with the RMSE at 0.7895, and M2 also consumes 1000 iterations with the RMSE at 0.7924. Both NLF and BNLF models converge with much lower RMSE than a WNMF does. Mover, according to Fig. 3(a), we see that the absolute reduction of learning objective (2) achieved by M3 is also much less than that achieved by M1-2 on D1, indicating that M1-2 can better approximate the learning objective than M3 does. The same situations are also found on D2-10.
- b) M1-2 enable their LF-distributions to converge to a steady-state. As shown in Fig. S1-2, M1-2's LFs initially distribute uniformly in the range of [0, 0.005] with a random hypothesis. However, their LF values and distributions change sharply during the first 200 iterations, and then change very slow during subsequent iterations, and finally converge to an equilibrium state. Such a phenomenon again supports our convergence proof.

D. Reconstruction Ability

In this part of the experiments, we validate M1-3's RMSE on Ψ of each dataset to see their reconstruction ability on an HiDS matrix. RMSEs of M1-3 on D1-10 are recorded in Table IV. Then we conduct the Friedman test [65] on these results to fully understand their significance.

The average ranks with each model's RMSE in table IV are computed in Table V. Let r_i^j denote the rank of the *j*th one of *p* tested models on the *i*th one of *S* testing cases, a Friedman test compares the average rank of each tested model calculated by

 $H_j = \sum_{i=1}^{s} r_i^j / S$. Then the Friedman value is computed as

$$\chi_F^2 = \frac{12S}{p(p+1)} \left[\sum_j H_j^2 - \frac{p(p+1)^2}{4} \right].$$
 (47)

Based on (47), the testing score is given by

$$F_F = \frac{(S-1)\chi_F^2}{S(p-1) - \chi_F^2},$$
(48)

which is distributed according to the *F*-distribution with p-1 and (p-1)(S-1) degrees of freedom [65]. Note that if F_F is larger than a given critical value α , the null hypothesis which claims the equivalence of all tested models can be rejected.

In our experiments, three models are tested on ten datasets. Hence, we have p=3 and S=10. Thus, F_F has (2, 18) degrees of freedom and the corresponding critical value is 3.55 for $\alpha=0.05$.

Hence, the null hypothesis can be rejected if the testing score is higher than 3.55. By substituting the average ranks of M1-3 in Table V into (47) and (48), we achieve that F_F =27.0, which is much higher than 3.55. Hence, M1-3 are significantly different with confidence at 95%.

TABLE IV RMSE of M1-3 on Ψ of D1-10.						
Dataset Model	D1	D2	D3	D4	D5	
M1	0.7901	0.8389	0.7258	0.9133	0.6101	
M2	0.7930	0.8417	0.7177	0.9114	0.5982	
M3	0.8498	0.8773	0.7655	0.9708	0.6481	
Dataset						
Model	D6	D7	D8	D9	D10	
M1	1.8517	0.2316	2.1359	0.1081	0.1409	
M2	1.8442	0.2335	2.0847	0.1126	0.1470	
M3	2.0781	0.2611	3.2824	0.1308	0.1667	
		_				

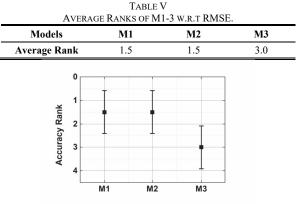


Fig. 5. Results of Nemenyi analysis

To further identify M1-3's performance, we adopt the Nemenyi test [65]. Two models are significantly different if the difference between their performance ranks is larger than the critical difference value [65] given by

$$CD = q_{\alpha} \sqrt{\frac{p(p+1)}{6S}}.$$
(49)

Note that q_a in (49) is 2.052 with the critical level α =0.1 as p=3 in our case [65]. By substituting p=3, S=10, and $q_{0,1}=2.052$ into (49), we obtain that CD=0.918. Hence, two models are significantly different in reconstruction ability on an HiDS matrix with the confidence of 90%, when their rank different value is larger than 0.918. The Nemenyi analysis results according to Tables IV and V are shown in Fig. 5. From them, we see that both M1 and M2, i.e., NLF and BNLF models, significantly outperform M3, i.e., a WNMF model, in terms of reconstruction ability on an HiDS matrix. In addition, M1 and M2 do not have a significance difference in the level of RMSE from each other.

E. Initialization Strategies

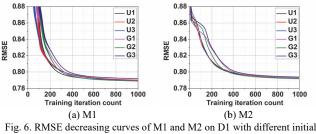
As revealed before [7]-[12], [26]-[31], [58], the performance of an NLF model is sensitive to its initial hypothesis. However, how to select an appropriate initial hypothesis for it remains an open issue. According to prior research [7]-[12], [26]-[31], [58], it is commonly accepted to randomly generate an initial hypothesis in the non-negative field of real numbers. Hence, it

is the distribution of these randomly generated initializations that affects the performance of a resultant model. For validating its effects, we have conducted tests with six different initialization distributions for M1-2. The details of tested initialization distributions are summarized in Table VI. TABLE VI

DETAILS OF TESTED DISTRIBUTIONS FOR GENERATING INITIAL HYPOTHESES OF M1-2. Note that F denotes all of their desired LFs. For M1, $F = \{A, X\}$,

	FOR M2, $F = \{B, C, A, X\}$.					
	No.	Distribution	No.	Distribution		
-	U1	<i>F~U</i> (0, 0.005)	G1	<i>F~N</i> (0.005, 1e-7)		
	U2	$F \sim U(0, 0.1)$	G2	<i>F~N</i> (0.1, 1e-5)		
-	U3	$F \sim U(0, 1.0)$	G3	$F \sim N(1.0, 1e-4)$		

The RMSE decreasing curves of M1-2 with different initialization distributions on D1 is depicted in Fig. 6. The RMSE of M1-2 when $F \sim U(0, 0.005)$ in 100 independent tests on D1 is depicted in Fig. 7. Note that similar results can be observed on D2-10. Table VII summarizes the RMSE of M1-2 on D1-3 with different initial hypotheses. From them, we see that:



hypotheses.

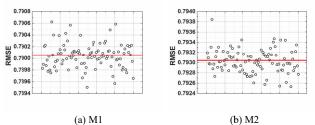


Fig. 7. RMSE of M1-2 when $F \sim U(0, 0.005)$ in 100 independent tests on D1. a) The prediction accuracy of an SLF-NMU-based NLF model is slightly affected by its initial hypothesis. From Fig. 6, we find that the convergence curves of M1-2 on D1 varies as their initialization distribution changes. However, they will always converge to an equilibrium point regardless of the initialization strategies. Moreover, from Fig. 7 we can only observe slight accuracy fluctuation of M1-2 by different

initial hypotheses randomly generated from the same distribution. The fluctuation ratio is limited in the range of

[-0.25%, 0.25%] according to our results. b) Appropriate initialization strategies can enable a more accurate model. If we aim at achieving performance gain via improving M1-2's initial hypothesis, the following two strategies can be considered: 1) choosing the initialization distribution wisely. According to Table VII, an NLF model with a Gaussian hypothesis mostly outperforms one with a Uniform hypothesis, which demonstrates that a Gaussian initialization distribution can probably improve an NLF model's prediction accuracy. But in practice, it is still necessary to adopt warming up tests with initialization

distributions on a probe set; and 2) building an ensemble. Since different initialization distributions can achieve diversified NLF models as shown in Fig. 6, they can form an efficient ensemble [57], [58] which can outperform any of its base models to achieve stably high accuracy.

 TABLE VII

 RMSE of M1-2 on D1-3 with Different Initial Hypotheses

		Uniform Hypothesis			Gaussian Hypothesis		
		U1	U2	U3	G1	G2	G3
D1	M1	0.7901	0.7905	0.7894	0.7901	0.7899	0.7930
D1	M2	0.7930	0.7930	0.7925	0.7923	0.7925	0.7947
D2	M1	0.8389	0.8389	0.8392	0.8387	0.8387	0.8392
D2	M2	0.8417	0.8419	0.8416	0.8414	0.8413	0.8417
D2	M1	0.7258	0.7226	0.7089	0.7423	0.7193	0.7359
D3	M2	0.7177	0.7158	0.7083	0.7177	0.7135	0.7283
-							

F. Summary

We summarize from the experimental results:

- a) An SLF-NMU-based NLF/BNLF model converges to a stable equilibrium point on an HiDS matrix;
- b) An SLF-NMU-based NLF/BNLF model converges better than an NMF model on an HiDS matrix. Its reconstruction ability for an HiDS matrix's unknown data is also better than that of an NMF Model; and
- c) An SLF-NMU-based NLF/BNLF model's regularization coefficient and initialization hypotheses should be chosen wisely to improve its performance.

V. DISCUSSIONS

A. Connections between an NLF and an NMF Model

An NMF model is designed for full matrices, which are mostly seen as images in the area of computer vision. Initially, Lee and Seung [30], [31] adopt it to extract local features from a non-negative matrix representing an image. Subsequently, many researchers investigate it and propose various NMF extensions [29]-[36], [48]-[52]. To achieve the desired non-negative feature matrices, a non-negative multiplicative update (NMU) algorithm is commonly adopted. With it, if $Y^{|M| \times |N|}$ is a full matrix, then it extracts features $A^{|M| \times d}$ and $X^{|N| \times d}$ as

$$a_{m,k} \leftarrow a_{m,k} \frac{\left(YX\right)_{m,k}}{\left(AX^{\mathsf{T}}X\right)_{m,k}}, x_{n,k} \leftarrow x_{n,k} \frac{\left(Y^{\mathsf{T}}A\right)_{n,k}}{\left(XA^{\mathsf{T}}A\right)_{n,k}}.$$
 (50)

As a matter of fact, other algorithms like the projected gradient descent [59], projected alternating least squares [60] are also proposed to train an NMF model. Nonetheless, an NMU algorithm does not make truncations during the training process, making it more suitable to represent the natural structures such as node clusters hiding in the original matrix. Meanwhile, it is implemented through making the learning rate adaptive to achieve the multiplicative form, i.e., its learning rate is self-adaptive. Hence, an NMF model frequently adopts an NMU algorithm. The processing flow of such a model is shown in Fig. S3 in the Supplementary File. According to (50), its computational complexity is $\Theta(|M| \times |N| \times k \times t)$ with t being training iteration count, and storage complexity is $\Theta(|M| \times |N|)$.

However, an NMF model cannot handle an HiDS matrix directly since the products YX and $Y^{T}A$ are intractable with Y being incomplete. As discussed in [28], [48], an NMF model

can be adjusted to fit an incomplete Y by integrating an indicator matrix $W^{|M| \times |N|}$ into (50) to achieve a weighted NMF (WNMF) model. In it, the indicator matrix's element is set at one if the corresponding element in Y is known, and zero otherwise. Thus, WNMF can extract non-negative features from an incomplete Y with an NMU algorithm:

$$a_{m,k} \leftarrow a_{m,k} \frac{\left((W \circ Y) X \right)_{m,k}}{\left(A X^{\mathrm{T}} X \right)_{m,k}}, x_{n,k} \leftarrow x_{n,k} \frac{\left((W \circ Y)^{\mathrm{T}} A \right)_{n,k}}{\left(X A^{\mathrm{T}} A \right)_{n,k}}; \quad (51)$$

where the operator \circ calculates the Hardamad product of two matrices. Thus, the products $(W \circ Y)X$ and $(W \circ Y)^T A$ are solvable when Y is HiDS. However, the computational and storage costs of WNMF are respectively $\Theta(|M| \times |N| \times k \times t)$ and $\Theta(|M| \times |N|)$, which are the same as those of NMF. It is compatible with existing NMF training algorithms like an NMF algorithm, however, it suffers unnecessarily high costs on an HiDS matrix. Its processing flow is in Fig. S4 in the Supplementary File.

In comparison, an NLF model is specifically designed for an HiDS matrix. With an SLF-NMU algorithm, its computational and storage costs are respectively $\Theta(|\Lambda| \times k \times t)$ and $\Theta(\max\{|\Lambda|, (|M|+|N|) \times d\})$. Thus, we have the following inferences:

$$\frac{T_{NLF}}{T_{NMF}} = \frac{|\Lambda| \times k \times t_{NLF}}{|M| \times |N| \times k \times t_{NMF}} \approx \frac{|\Lambda|}{|M| \times |N|}$$

$$\frac{S_{NLF}}{S_{NMF}} = \frac{max \left\{ |\Lambda|, \ (|M|+|N|) \times d \right\}}{|M| \times |N|} = max \left\{ \frac{|\Lambda|}{|M| \times |N|}, \ d\left(\frac{1}{|M|} + \frac{1}{|N|}\right) \right\}$$
(52)

Given that $|\Lambda| \ll |M| \times |N|$, i.e., the known data of an HiDS matrix are far less than its unknown ones (e.g., the known data of the NetFlix matrix take 0.21% of its all entries only), an SLF-NMU-based NLF model's computational and storage costs are much lower than those of an NMF model in theory. Hence, an NLF model is far more efficient than an NMF-type model on an HiDS matrix. Its processing flow is depicted in Fig. S5 in the Supplementary File. From this point of view, it is much suitable to address an HiDS matrix than an NMF model does on the premise that it converges well, which is guaranteed by the convergence analysis given in this paper.

On the other hand, it is well known that in the area of recommender systems or social network services, an HiDS matrix is far more frequently encountered than a full one. Therefore, we'd prefer to take an NMF model as a special case for an NLF model owing to the following reasons:

- a) In our concerned big data-related Web-applications like a recommender system, the observed data are commonly incomplete, making an HiDS matrix be far more frequently encountered than a full matrix. Actually, a full matrix can be considered as an HiDS matrix whose data density is 100% in such a scenario, indicating that the interactions among users and items are fully observed (or quantized by the system, which is also an ultimate objective for a recommender system); and
- b) Note that owing to its data-density-oriented learning objective and algorithm, i.e., an SLF-NMU algorithm, an NLF model can address an HiDS matrix whose data density can be an arbitrary number in the (0%, 100%] interval. In other words, it can address a matrix with/without missing data. In comparison, an NMF model is defined on a full matrix. Thus, it can only handle a matrix without missing

data (or transmit a HiDS target into a full one like in a WNMF model).

Nonetheless, in other fields like computer vision, full matrices representing normal images are much more than incomplete ones. Under such circumstances, an NLF model can be considered as a special case of an NMF model. From this point of view, we clearly see that although these two kinds of models are closely connected, they are targeting at different problems. It is important to make an appropriate choice for a specific problem. From the theoretical and empirical studies of this paper, it is efficient to adopt NLF on an HiDS matrix.

B. Theoretical Achievements of This Study

Since both NMF and NLF models are bi-linear, an auxiliary function-based method can be adopted to show that both NMU for NMF and SLF-NMU for NLF make their loss functions non-increasing. Nonetheless, the theoretical achievements of this work stand in two aspects: 1) an SLF-NMU is single LF-dependent, making its mathematical expression very different from that of an NMU algorithm. Meanwhile, an HiDS matrix's data density is low and distribution is highly imbalanced. The convergence analysis in this paper innovatively shows that an SLF-NMU learning algorithm can enable an NLF model to converge on an arbitrary matrix in spite of its sparsity and imbalanced data distribution; 2) its ability to converge to a KKT equilibrium point is also proved on an HiDS matrix, which is also not seen in prior studies.

C. Local or Global Convergence

It should be mentioend that the objective function of an NLF/BNLF model is constrained and non-convex. Meanwhile, according to (6), an SLF-NMU-based learning algorithm actually implements an additive gradient descent-based training process with carefully-selected learning rates to guarantee the non-negativity of a resultant model. In other words, its achieved stationary point (whose properties are verified according to the previously provided theoretical studies) is a first-order one on a non-convex problem. According to a prior study [25], such a first-order stationary point can be a global optimum, local optimum, or saddle point. How to identify its more specific properties is very challenging (which still remains unveiled in the optimization community according to [25]). We plan to address this problem in our future work.

VI. CONCLUSIONS

In this paper, we rigorously prove that an NLF/BNLF model defined on an HiDS matrix converges to a KKT equilibrium point of its objective with an SLF-NMU-based learning algorithm. Note that the proof consists of two steps, a) proving that its learning objective goes non-increasing with SLF-NMU by constructing a specifically-designed auxiliary function; and b) proving that its parameter learning sequences finally converge to a stable equilibrium point with SLF-NMU by analyzing the KKT conditions of its learning objective.

Note that this study conducts the convergence analysis on an objective relying on the Euclidean distance. However, the same principle also applies equally to an NLF model depending on other kinds of loss functions. With it, an SLF-NMU-based NLF model's convergence characteristics are theoretically justified, which are also supported by the empirical results on ten HiDS matrices from real applications.

As revealed in previous studies [3], the parallelization of an SLF-NMU algorithm can be implemented via a properly-designed distributed computing framework. In this case, can it still converge to a stable equilibrium point? We will answer this question in the future.

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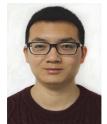
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