Convergence to Second-Order Stationarity for Non-negative Matrix Factorization: Provably and Concurrently

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Abstract

Non-negative matrix factorization (NMF) is a fundamental non-convex optimization problem with numerous applications in Machine Learning (music analysis, document clustering, speech-source separation etc). Despite having received extensive study, it is poorly understood whether or not there exist natural algorithms that can provably converge to a local minimum. Part of the reason is because the objective is heavily symmetric and its gradient is not Lipschitz. In this paper we define a multiplicative weight update type dynamics (modification of the seminal Lee-Seung algorithm) that runs concurrently and provably avoids saddle points (first order stationary points that are not second order). Our techniques combine tools from dynamical systems such as stability and exploit the geometry of the NMF objective by reducing the standard NMF formulation over the non-negative orthant to a new formulation over a scaled simplex. An important advantage of our method is the use of concurrent updates, which permits implementations in parallel computing environments.

1 Introduction

Consider a non-negative data matrix $V \in \mathbb{R}^{n \times m}_{\geq 0}$ consisting of $m$ samples each with $n$ non-negative features, arranged as its columns. In the non-negative matrix factorization (NMF) problem the goal is to identify two entrywise non-negative matrices $W \in \mathbb{R}^{n \times r}_{\geq 0}$ and $H \in \mathbb{R}^{r \times m}_{\geq 0}$ (for some a-priori fixed $r \in \mathbb{N}$) such that the matrix product $WH$ approximates $V$, where the precise sense of approximation depends on the application of interest.

Factorizations based on non-negative matrices have found numerous applications throughout most fields of science and engineering, notable examples including music analysis [7], document clustering [36], speech-source separation [34] and cancer-class identification [9]. NMFs are useful as they lead to additive and sparse representations of the input data. Indeed, a factorization $V = WH$ can be interpreted as $V(:,j) = WH(:,j)$, for all $j = 1, \ldots, m$, i.e., each sample (columns of $V$) can be represented as non-negative combination of basis vectors (columns of $W$).

The NMF problem was introduced in the engineering community in the seminal paper [30] and was subsequently popularized further in [21]. As it turns out, non-negative factorizations were also explored earlier in the combinatorial optimization community, as a tool to describe the efficacy of linear programming for hard combinatorial problems [37].

In terms of complexity, the problem of deciding the existence of an exact NMF is NP-hard even for $r = \text{rank}(V)$ [35]. [5] gave the first finite algorithm for calculating the non-negative rank
over the real numbers based on quantifier elimination arguments. Extending this technique, [33] derived an \((mn)^{O(2^r)}\) algorithm for exact NMF that was subsequently improved to \((2^r mn)^{O(r^2)}\) [27]. Additionally, [33] identified sufficient conditions on \(V\) under which the NMF problem can be solved in polynomial time.

There are several practically efficient algorithms for calculating (approximate) NMFs. The starting point for the majority of existing approaches is the non-convex program

\[
\min_{W \in \mathbb{R}_+^{n \times r}, H \in \mathbb{R}_+^{r \times m}} F(W, H) := \|V - WH\|_F^2,
\]

for some user-specified parameter \(r \in \mathbb{N}\). Nevertheless, in many applications, it is useful to use information-theoretic divergences rather than the squared Euclidean loss function. In view of the non-convexity of \((\text{NMF})\), the theoretical analysis of iterative algorithms for solving \((\text{NMF})\) typically amounts to showing that an accumulation point of the sequence of iterates \((W_t, H_t)\) generated by the algorithm satisfies the first-order optimality conditions given in (1).

Many algorithms for NMF can be interpreted in a unified manner within the framework of block coordinate descent (BCD), which is also known as the Gauss-Seidel method, e.g., see the survey [20] and references therein. In the BCD framework the goal is to minimize a smooth function over a domain that can be decomposed as the Cartesian product of closed convex sets. At each iteration of the BCD method, the function is minimized with respect to a single block of variables while the rest of the blocks are kept fixed. Convergence results in the BCD framework typically require attainment and unicity of the minimizer at each step [3], the unicity assumption being redundant in the 2-block case [14]. One example is the Alternating Non-negative Least Squares (ANLS) method [19], which is a 2-block BCD with updates given by the solutions of \(\min_{W \geq 0} \|V - WH\|^2\), and \(\min_{H \geq 0} \|V - WH\|^2\). A second example is the Hierarchical ALS (HALS) method [1], which has been rediscovered several times, e.g. as the rank-one residue iteration [15] and FastNMF in [24]. The HALS method corresponds to a \(2r\)-block BCD, one for each column of the factors \(W\) and \(H\). For additional details concerning algorithms for NMF and their convergence properties the reader is referred to the surveys [20, 12] and references therein.

Going beyond the BCD framework, the multiplicative update (MU) rule introduced in [22] is by far the most popular algorithm for NMF. In the MU framework, the updates are given by

\[
W_{t+1} = W_t \odot \frac{V H_t^T}{W_t H_t H_t^T} \quad H_{t+1} = H_t \odot \frac{W_{t+1}^T V}{W_{t+1}^T W_{t+1} H_t},
\]

where \(X/Y\) denotes the componentwise division of two matrices. [22] showed using a majorization-minimization approach, e.g., see [38], that under the MU rule, the objective function \(\|V - WH\|_F^2\) is non-increasing. However, it has long been observed that the MU rule may fail to converge to a first-order stationary point, e.g. see [13]. Indeed, only when the MU method converges to a fixed point \((W, H)\) with strictly positive entries this is also a KKT point. An important limitation of the MU update rule is that it cannot be implemented concurrently (as \(H_{t+1}\) depends on \(W_{t+1}\)). [25] further elaborates on the difficulties in proving convergence of the MU algorithm, while establishing convergence of a close variant of Lee-Seung’s method.

Despite the wealth of existing algorithmic approaches for finding NMFs, a common limitation is that they may fail to avoid saddle points, e.g. see [8, 13, 17, 4, 2]. This drawback is also shared with many gradient-based approaches applied to important optimization problems (e.g. training neural networks, matrix completion, community detection), as such methods are only guaranteed to converge to first-order stationary points, among which there exists a proliferation of highly-suboptimal saddle points, e.g., see [6]. At the same time, algorithmic approaches that
incorporate additional curvature information typically converge to second-order stationary points, i.e., points with vanishing gradient and positive semidefinite Hessian, which turn out to be as good as local minima in many problems of practical interest [11]. These observations have led to a flurry of research activity on avoiding saddle points the last 5 years (see [10, 23, 18, 32, 31, 28] and references therein) for both unconstrained and constrained optimization. One other line of work that deals with avoiding saddle points in non-convex settings with linear constraints and can be applied to our paper (as long as one has shown our main Theorem 2) can be found in [29, 26]. Our main goal in this work is to identify new methods that converge to second-order stationary points of (NMF).

1.1 Summary of results and significance

Before we formally state our results, we provide some standard definitions in constrained optimization applied to the NMF problem (NMF). Moreover, we give the definition of our Multiplicative Weights Update (MWU) applied to NMF.

Stationary points of (NMF). A pair of matrices \((W^*, H^*)\) is a first-order stationary point (FOSP) of problem (NMF) if for all \(i \in [n], k \in [r], j \in [m]\) it satisfies:

\[
\begin{align*}
W_{ik}^*, H_{kj}^* &\geq 0, \\
W_{ik}^* > 0 &\implies \frac{\partial F(W^*, H^*)}{\partial W_{ik}} = 0, \\
H_{kj}^* > 0 &\implies \frac{\partial F(W^*, H^*)}{\partial H_{kj}} = 0, \\
W_{ik}^* = 0 &\implies \frac{\partial F(W^*, H^*)}{\partial W_{ik}} \geq 0, \\
H_{kj}^* = 0 &\implies \frac{\partial F(W^*, H^*)}{\partial H_{kj}} \geq 0.
\end{align*}
\]

(1)

Additionally, \((W^*, H^*)\) is a second-order stationary point (SOSP) of the problem (NMF) if it is a FOSP, and moreover,

\[
(\text{vec}(W)^\top, \text{vec}(H)^\top)\nabla^2 F(W^*, H^*) \left( \begin{array}{c} \text{vec}(W) \\ \text{vec}(H) \end{array} \right) \succeq 0,
\]

(2)

for any pair of matrices \((W, H)\) satisfying:

\[
\begin{align*}
\frac{\partial F(W^*, H^*)}{\partial W_{ik}} > 0 &\implies W_{ik} = 0, \quad W_{ik}^* = 0 \implies W_{ik} \geq 0, \\
\frac{\partial F(W^*, H^*)}{\partial H_{kj}} > 0 &\implies H_{kj} = 0, \quad H_{kj}^* = 0 \implies H_{kj} \geq 0,
\end{align*}
\]

for all \(i \in [n], k \in [r], j \in [m]\).

We now present our multiplicative weight update method, which converges to a SOSP of (NMF) with probability 1.

Denote by \(S\) the set of fixed points of MWU dynamics/algorithm (1), namely the set of points \((W, H)\) that are invariant under the update rule of MWU, multiplied by scalar \(C\). Then, the set of stationary points of problem (NMF) with the additional constraint that \(\sum_{i,j} W_{ij} + \sum_{i,j} H_{ij} = C\) is a subset of \(S\).
Algorithm 1 Concurrent Multiplicative Weight Update

Input: A matrix $V_{n \times m}$ with positive elements

Output: Matrices $W_{n \times r}, H_{r \times m}$ s.t. $V \simeq W \cdot H$.

$C = 4r(nm)^{1/4} \sqrt{\|V\|_F}$, $\epsilon = \Theta(\frac{1}{C^2})$

$(W_0, H_0) \leftarrow$ a random point in simplex

$V \leftarrow V/C^2$

for $t = 1$ to $T$

$W_{t+1}^{ik} = W_t^{ik} \cdot (1 - \epsilon \cdot \frac{\partial F(W_t, H_t)}{\partial W_{ik}})/Z$

$H_{t+1}^{kj} = H_t^{kj} \cdot (1 - \epsilon \cdot \frac{\partial F(W_t, H_t)}{\partial H_{kj}})/Z$

$Z = 1 - \epsilon \cdot \left( \sum_{i,k} W_t^{ik} \cdot \frac{\partial F(W_t, H_t)}{\partial W_{ik}} + \sum_{k,j} H_t^{kj} \cdot \frac{\partial F(W_t, H_t)}{\partial H_{kj}} \right)$

end for

return $W \leftarrow C \cdot W^{T+1}, H \leftarrow C \cdot H^{T+1}$

We now state the main result of our paper, which informally states that the MWU dynamics (1) provably avoids fixed points that are not second order stationary points.

Main Theorem. The MWU described in Algorithm 1 converges to the set of fixed points for any initialization $(W^0, H^0) \in \Delta_{nr+rm}$. Moreover, the set of initial conditions so that MWU converges to a point $(\tilde{W}, \tilde{H})$ for which $(W^*, H^*) := C \cdot (\tilde{W}, \tilde{H})$ is not a second order stationary point for problem (NMF) is of measure zero (in $\Delta_{nr+rm}$).

An immediate corollary is the following:

Corollary 1. Assume that the iterate $(W^t, H^t)$ converges to a limit, under random initialization (any probability distribution that is absolutely continuous with respect to Lebesgue measure on $\Delta_{nr+rm}$ suffices for the initialization) the probability of MWU (1) to converge to a point $(\tilde{W}, \tilde{H})$ so that $(W^*, H^*) := C \cdot (\tilde{W}, \tilde{H})$ is a second order stationary point for problem (NMF) is one.

An important differentiation between the concurrent MWU rule and existing MWUs and gradient based approaches, is the concurrent way of updating the entries of $W$ and $H$. Both iterates $W_t^{t+1}$ and $H_t^{t+1}$ are updated using only the values of $W_t$ and $H_t$, an extremely useful algorithmic feature since it permits implementations in parallel computing environments. To the best of our knowledge, Algorithm 1 is the first iterative method for NMF that converges while performing its updates in a concurrent way. In all previous gradient based approaches (both in multiplicative weight algorithms and in alternating least squares) the convergence properties heavily rely on the fact that the entries of $W$ and $H$ are updating in an alternating way, while their concurrent counterparts may fail to converge. Such an instance is presented in Example 1 for the Lee-Seung algorithm.

1.2 Proof techniques

The main challenge in the non-convex problem of NMF is that the landscape is not Lipschitz (in the positive orthant) and there are continuums of stationary points (if $W, H$ is a stationary point, so it is $WD, D^{-1}H$ with $D$ a diagonal matrix with positive entries). The first challenge is essentially circumvented by adding an extra linear constraint that makes the feasibility region a compact set. In particular we define a modification of the NMF problem with the extra constraint that the sum of the entries of $W$ and $H$ is equal to a specific constant $C$ sufficiently large (this constant is chosen to be $C > 2 \cdot r \cdot (nm)^{1/4} \sqrt{\|V\|_F}$). By choosing this constant that large, we are able to prove that all the fixed points of MWU that are not second order stationary points of the NMF problem are
repelling for MWU inside simplex. Moreover, we are able to show that for any stationary point \((W^*, H^*)\) of NMF, there exists another stationary point \(\tilde{W}, \tilde{H}\) so that \(W^*H^* = \tilde{W}\tilde{H}\) and the sum of entries of \(\tilde{W}\) and \(\tilde{H}\) is exactly \(C\). As long as we have shown these claims, we use a result from [32] (Theorem 1) that states that given any twice differentiable polynomial function \(f(x)\) that we want to maximize with simplex constraints, MWU dynamics converges to second order stationary points almost surely. Last but not least, we can show that after adding the simplicial constraint (that is the sum of entries of \(W, H\) must be equal to \(C\)) for any stationary point \((W^*, H^*)\) of the classic NMF problem there exists a stationary point \((\tilde{W}, \tilde{H})\) such that \(F(W^*, H^*) = F(\tilde{W}, \tilde{H})\) (they have same values) and moreover \((\tilde{W}, \tilde{H})\) lies in the positive orthant and satisfies the aforementioned simplicial constraint (see Lemma 1).

**Notation.** We use \(W_{i}^{t}\) to denote the \(i\)-th column of matrix \(W\) and \(H_{i}^{t}\) to denote the \(i\)-th row of matrix \(H\). We also use subscripts or superscripts with letter \(t\) to denote the \(t\)-th iterate. We denote by \(\text{vec}(A)\) the standard vectorization of matrix \(A\), by \([n]\) the set \(\{1, 2, ..., n\}\) and by \(\Delta_n\) the simplex of size \(n\), that is \(\Delta_n = \{x \in \mathbb{R}^n : x \geq 0, \sum_{i=1}^{n} x_i = 1\}\).

# 2 Non-negative matrix factorization under simplicial constraints

Before giving the details of our proof, we elaborate the strong relation between Algorithm 1 and the following optimization problem, which we call simplex-NMF:

\[
\begin{align*}
\min & \quad \|V - WH\|_F^2, \\
\text{s.t.} & \quad \sum_{i,k} W_{ik} + \sum_{k,j} H_{kj} = C \\
& \quad W \in \mathbb{R}_{+}^{n \times r}, H \in \mathbb{R}_{+}^{r \times m}, \quad (S-NMF)
\end{align*}
\]

where \(C\) is any constant \(> 2r(nm)^{1/4} \sqrt{\|V\|_F}\).

Problem \((S-NMF)\) is similar to the original NMF problem, the only difference being the additional simplex constraint. On the negative side, the feasibility set of \((S-NMF)\) is a strict subset of the feasibility set of the original NMF problem, meaning that it may include solutions with cost much greater than the optimal value of the original NMF problem. On the positive side, this problem turns out to be algorithmically easier to tackle. More precisely, due to the recent result [32], when \(C > 2r(nm)^{1/4} \sqrt{\|V\|_F}\) the sequence of matrices generated by the MWU algorithm will converge almost surely to a SOSP of \((S-NMF)\).

**Stationary points of \((S-NMF)\).** A pair of matrices \((W^*, H^*)\) is a first-order stationary point of the problem \((S-NMF)\) if for all \(i \in [n], j \in [m], k \in [r]\), we have:

\[
\begin{align*}
W^*_{ik}, H^*_{kj} & \geq 0, \\
\sum_{i,k} W^*_{ik} + \sum_{k,j} H^*_{kj} & = C, \\
W^*_{ik} > 0 & \implies \frac{\partial F(W^*, H^*)}{\partial W_{ij}} = c, \quad \text{for } i \in [n], k \in [r] \\
H^*_{kj} > 0 & \implies \frac{\partial F(W^*, H^*)}{\partial H_{kj}} = c, \quad \text{for } k \in [r], j \in [m]
\end{align*}
\]
\[ W_{ik}^* = 0 \implies \frac{\partial F(W^*, H^*)}{\partial W_{ik}} \geq c, \text{ for } i \in [n], k \in [r] \]
\[ H_{kj}^* = 0 \implies \frac{\partial F(W^*, H^*)}{\partial H_{kj}} \geq c, \text{ for } k \in [r], j \in [m] \]
for some constant \( c \). Additionally, a pair of matrices \((W^*, H^*)\) is a second-order stationary of the problem (S-NMF) if it is a FOSP, and moreover,

\[
(\text{vec}(W)^\top, \text{vec}(H)^\top) \nabla^2 F(W^*, H^*) \left( \begin{array}{c}
\text{vec}(W) \\
\text{vec}(H)
\end{array} \right) \geq 0,
\]

for any pair of matrices \((W, H)\) satisfying:

\[
\frac{\partial F(W^*, H^*)}{\partial W_{ik}} > c \implies W_{ik} = 0, \quad W_{ik}^* = 0 \implies W_{ik} \geq 0,
\]
\[
\frac{\partial F(W^*, H^*)}{\partial H_{kj}} > c \implies H_{kj} = 0, \quad H_{kj}^* = 0 \implies H_{kj} \geq 0,
\]
\[
\sum_{i=1}^{n} \sum_{k=1}^{r} W_{ik} + \sum_{j=1}^{m} \sum_{k=1}^{r} H_{kj} = 0.
\]

**Theorem 1** ([32]). Consider the problem \( \max \{ Q(x) : x \in \Delta_d \} \) where \( Q : \mathbb{R}^d \to \mathbb{R} \) is a polynomial function. Then, the MWU algorithm with update rule

\[
x_{i}^{t+1} = x_{i}^{t} \frac{1 + \epsilon \frac{\partial Q}{\partial x_{i}}}{1 + \epsilon \sum_{j} \frac{\partial Q}{\partial x_{j}}} \text{ for all } i \in [d],
\]

has the property that \( Q(x_{i}^{t+1}) > Q(x_{i}^{t}) \) unless \( x_{i}^{t} \) is a fixed point of the MWU dynamics (5). Moreover, the set of initial conditions so that the MWU dynamics (5) converge to a point that is not a second order stationary point for \( \max \{ Q(x) : x \in \Delta_d \} \) is of measure zero. The statement holds when \( \epsilon \) is chosen to be of order \( \Theta(1/C^2) \) (see also Algorithm 1).

Notice that the MWU described in Algorithm 1 is the same with the MWU of Theorem 1 applied for \( Q := -F \) (make it a minimization problem). Also observe that, \( F \) can be described as multivariate polynomial and thus Theorem 1 applies if the parameter \( \epsilon \) is selected appropriately small. For our case, \( \epsilon \) should be \( \Theta(1/C^2) \) (see also Algorithm 1).

To this end, Theorem 1 ensures that the MWU algorithm (almost certainly) converges to a SOSP of (S-NMF). However there is no reason why one should be interested in finding such points, since these points are not necessarily SOSPs of (NMF). In fact, a SOSP of (S-NMF) can be an arbitrarily bad solution for the initial NMF problem (e.g. consider the case \( C = 0 \)). One of our main technical contributions consists in showing that if the offset \( C \) exceeds a certain threshold (depending on \( n, m, r, \|V\|_F \)) then the set of SOSPs of (S-NMF) is a subset of the second-order stationary points of (NMF). Specifically, we show that:

**Theorem 2.** For any \( C > 2r(nm)^\frac{1}{2} \sqrt{\|V\|_F} \) we have that

- The value of (S-NMF) is equal to (NMF).
- Any second-order stationary point of (S-NMF) is also a second-order stationary point of (NMF).
The proof of the main theorem follows easily by combining Theorem 2 with Theorem 1. The first part of Theorem 2 is a consequence of the following result, proven in Section 3.

**Lemma 1.** For any first-order stationary point of (NMF) there exists a first-order stationary point of (S-NMF) with the same value.

The second part of Theorem 2 heavily relies on the following result, which is proven in Section 4.

**Lemma 2.** Any second-order stationary point of the problem (S-NMF) necessarily satisfies $c = 0$. In particular, any second-order stationary point of (S-NMF) is a first-order stationary point of (NMF).

Lastly, note that Lemma 2 combined with Theorem 1 imply the following claim: If we apply the MWU to problem (S-NMF) with $C > 2r(nm)^{4} \sqrt{\|V\|_F}$, the generated sequence of matrices will converge (almost certainly) to a pair of matrices $(W^*, H^*)$ that is a FOSP of the problem (NMF). Although the latter claim is not enough for our initial goal (finding pair of matrices that are second-order stationary points for NMF (2)), it is the basic step of the proof of Theorem 2, that is presented in Section 5.

In Section 6, we present the results of several experimental evaluations indicating that the MWU defined in Algorithm 1 converges to the optimal pair of matrices.

### 2.1 An illustrative example

Before proceeding we exhibit the above discussion in a very simple but illustrative example. Consider the following instance of the NMF problem:

$$\min \{(1 - xy)^{2} : x, y \geq 0\}.$$  

For the above optimization problem the set of first-order stationary points (Equation (1)) is the union of the sets, $\{(x, 0) : x \geq 0\}, \{(0, y) : y \geq 0\}, \{(x, y) : x \cdot y = 1, x \geq 0, y \geq 0\}$. While the set of the second-order stationary points (Equation (2)) is just the set $\{(x, y) : x \cdot y = 1, x \geq 0, y \geq 0\}$. This simple example indicates the interest in finding second-order stationary points (Equation (2)) since the set of first order stationary points (Equation (1)) contains very bad solutions.

Now consider the same problem with an additional simplicial constraint:

$$\min \{(1 - xy)^{2} : x + y = 1, x, y \geq 0\}.$$  

In this case the set of first-order stationary points (Equation (3)) is $\{(0, 1), (1, 0), (1/2, 1/2)\}$. While the set of second order stationary points (Equation (4)) is the set $\{(1/2, 1/2)\}$. The above means that if we run the MWU algorithm runs with parameter $C = 1$ then for almost all initializations, the produced sequence of solutions will converge to $(1/2, 1/2)$, since this is the only second-order stationary point of the above minimization problem. Now notice that $(1/2, 1/2)$ is not a good solution (for the initial optimization problem), the value of the global optimal (for the initial optimization problem) is 0. More importantly, the point $(1/2, 1/2)$ does not satisfy Equation (2), which was our initial algorithmic goal. The reason for this is that the parameter $C$ is not chosen large enough (notice that $C$ must be selected as $2r(nm)^{4} \sqrt{\|V\|_F}$ which is greater than 1) and thus Theorem 2 does not apply.

Now consider the problem with the same additional simplicial constraint, but with $C = 4$.

$$\min \{(1 - xy)^{2} : x + y = 4, x, y \geq 0\}.$$  

In this case the set of first-order stationary points (Equation (3)) is \( \{(0, 1), (1, 0), (2, 2), (2 - \sqrt{3}, 2 + \sqrt{3}), (2 + \sqrt{3}, 2 - \sqrt{3})\} \). While the set of second order stationary points (Equation (4)) is \( \{(2 - \sqrt{3}, 2 + \sqrt{3}), (2 + \sqrt{3}, 2 - \sqrt{3})\} \). As a result, MWU algorithm with parameter \( C = 4 \) converge either to \((2 - \sqrt{3}, 2 + \sqrt{3})\) or to \((2 + \sqrt{3}, 2 - \sqrt{3})\) for almost all initializations. Notice that both \((2 - \sqrt{3}, 2 + \sqrt{3})\) and \((2 + \sqrt{3}, 2 - \sqrt{3})\) satisfy Equation (2) (in fact they are optimal solutions). This should not be a surprise since for \( C = 4 \), Theorem 2 applies and thus MWU converges to second-order stationary points of Equation (2).

### 2.2 Calculating derivatives

The entries of the gradient of \( F \) are given by:

\[
\frac{\partial F}{\partial W_{ik}} = -2 \sum_{j=1}^{m} \left( V_{ij} - \sum_{\ell=1}^{r} W_{i\ell} H_{\ell j} \right) H_{kj},
\]

\[
\frac{\partial F}{\partial H_{kj}} = -2 \sum_{i=1}^{n} \left( V_{ij} - \sum_{\ell=1}^{r} W_{i\ell} H_{\ell j} \right) W_{ik},
\]

whereas the entries of its Hessian are given by:

\[
\frac{\partial^2 F}{\partial^2 W_{ik}} = 2 \sum_{j=1}^{m} H_{kj}^2 \quad \text{and} \quad \frac{\partial^2 F}{\partial^2 H_{kj}} = 2 \sum_{i=1}^{n} W_{ik}^2
\]

\[
\frac{\partial^2 F}{\partial W_{ik} \partial W_{i'\ell}} = 0 \quad \text{and} \quad \frac{\partial^2 F}{\partial H_{kj} \partial H_{\ell j'}} = 0 \quad \text{for} \quad i \neq i', j \neq j'
\]

\[
\frac{\partial^2 F}{\partial W_{ik} \partial H_{kj}} = 2 \sum_{j=1}^{m} H_{kj} H_{kj}
\]

\[
\frac{\partial^2 F}{\partial H_{kj} \partial H_{\ell j}} = 2 \sum_{i=1}^{n} W_{i\ell} W_{ik}
\]

\[
\frac{\partial^2 F}{\partial W_{ik} \partial H_{kj}} = -2V_{ij} + 2 \sum_{\ell=1}^{r} W_{i\ell} H_{\ell j} + 2W_{ik} H_{kj}
\]

\[
\frac{\partial^2 F}{\partial W_{ik} \partial H_{\ell j}} = 2W_{i\ell} H_{kj}.
\]

Using (6) and (7) we arrive at the following useful result:

**Lemma 3.** For any pair of matrices \( (W, H) \) and index \( k \in \{1, \ldots, r\} \), let the pair of matrices \( (\tilde{W}, \tilde{H}) \) such that 1) \( \tilde{W}_{ik} = W_{ik} \) and \( \tilde{W}_{i\ell} = 0 \), 2) \( \tilde{H}_{kj} = -H_{kj} \) and \( \tilde{H}_{\ell j} = 0 \). Then

\[
(\text{vec}(\tilde{W})^\top, \text{vec}(\tilde{H})^\top) \cdot \nabla^2 F(W, H) = \begin{pmatrix}
0^\top \\
-\nabla_Wk F \\
0^\top \\
\nabla_{Hkj} F \\
0^\top
\end{pmatrix},
\]

where \( 0 \) denotes the zero column vector of appropriate size.

**Proof.** Let us start by proving that for all the entries of the vector corresponding respectively to \( W_{ik} \) and \( H_{kj} \),
• \[ \left[ \text{vec}(\mathbf{W})^\top, \text{vec}(\mathbf{H})^\top \right] \cdot \nabla^2 F(W, H) \] 

\[ W_{ik} = -\frac{\partial F}{\partial W_{ik}} \]

• \[ \left[ \text{vec}(\mathbf{W})^\top, \text{vec}(\mathbf{H})^\top \right] \cdot \nabla^2 F(W, H) \] 

\[ H_{kj} = \frac{\partial F}{\partial H_{kj}} \]

By direct calculation we get that,

\[ \left[ \text{vec}(\mathbf{W})^\top, \text{vec}(\mathbf{H})^\top \right] \cdot \nabla^2 F(W, H) \]

\[ W_{ik} = \frac{\partial^2 F}{\partial^2 W_{ik}} \mathbf{W}_{ik} + 2 \sum_{\ell \neq k} \frac{\partial^2 F}{\partial W_{ik} \partial W_{i\ell}} \mathbf{W}_{i\ell} + 2 \sum_{j=1}^{m} \frac{\partial^2 F}{\partial W_{ik} \partial H_{kj}} \hat{H}_{kj} \]

\[ = \frac{\partial^2 F}{\partial^2 W_{ik}} \mathbf{W}_{ik} + 2 \sum_{j=1}^{m} \frac{\partial^2 F}{\partial W_{ik} \partial H_{kj}} \hat{H}_{kj} \]

\[ = \frac{\partial^2 F}{\partial^2 W_{ik}} \mathbf{W}_{ik} + 2 \sum_{j=1}^{m} \frac{\partial^2 F}{\partial W_{ik} \partial H_{kj}} (-H_{kj}) \]

\[ = 2 \sum_{j=1}^{m} W_{ik} H_{kj}^2 + 2 \sum_{j=1}^{m} \left[ V_{ij} - \sum_{\ell=1}^{r} W_{i\ell} H_{\ell j} \right] H_{kj} - 2 \sum_{j=1}^{m} W_{ik} H_{kj}^2 \]

\[ = -\frac{\partial F}{\partial W_{ik}} \]

where the last equality follows by (6). Respectively for \( H_{kj} \). Up next we prove that

\[ \left[ \text{vec}(\mathbf{W})^\top, \text{vec}(\mathbf{H})^\top \right] \cdot \nabla^2 F(W, H) \]

\[ W_{ik'} = \left[ \text{vec}(\mathbf{W})^\top, \text{vec}(\mathbf{H})^\top \right] \cdot \nabla^2 F(W, H) \]

\[ H_{kj'} = 0 \]

\[ \left[ \text{vec}(\mathbf{W})^\top, \text{vec}(\mathbf{H})^\top \right] \cdot \nabla^2 F(W, H) \]

\[ W_{ik'} = \frac{\partial^2 F}{\partial^2 W_{ik'}} \mathbf{W}_{ik'} + 2 \sum_{\ell \neq k'} \frac{\partial^2 F}{\partial W_{ik'} \partial W_{i\ell}} \mathbf{W}_{i\ell} + 2 \sum_{j=1}^{m} \frac{\partial^2 F}{\partial W_{ik'} \partial H_{k'j}} \hat{H}_{k'j} \]

\[ = 2 \sum_{j=1}^{m} \frac{\partial^2 F}{\partial W_{ik'} \partial W_{ik}} \mathbf{W}_{ik} + 2 \sum_{j=1}^{m} \frac{\partial^2 F}{\partial W_{ik'} \partial H_{kj}} \hat{H}_{kj} \]

\[ = 2 \sum_{j=1}^{m} \frac{\partial^2 F}{\partial W_{ik'} \partial W_{ik}} \mathbf{W}_{ik} + 2 \sum_{j=1}^{m} \frac{\partial^2 F}{\partial W_{ik'} \partial H_{kj}} (-H_{kj}) \]

\[ = 2 \sum_{j=1}^{m} H_{k'j} H_{kj} W_{ik} - 2 \sum_{j=1}^{m} W_{ik} H_{k'j} H_{kj} = 0. \]

Respectively for \( H_{k'j} \). \( \square \)
3 Proof of Lemma 1

By Theorem 6, [16], any FOSP \((W^*, H^*)\) of the problem (NMF) satisfies \(\|W^*H^*\|_F \leq \|V\|_F\).

Consider the pair matrices \((\hat{W}, \hat{H})\) defined by:

\[
\hat{W}^k = \sqrt{\frac{\|H^*_k\|_1}{\|W^*k\|_1}} W^*k \quad \text{and} \quad \hat{H}_k = \sqrt{\frac{\|W^*k\|_1}{\|H^*_k\|_1}} H^*_k,
\]

for each \(k \in [r]\). Without loss of generality we assumed that both \(\|W^*k\|_1\) and \(\|H^*_k\|_1\) are not equal to zero (if one of these terms is zero, we may assume and the other is also zero and the inequality below still holds). By definition of \((\hat{W}, \hat{H})\) we have that

\[
\hat{W} \hat{H} = \sum_{k=1}^{r} \hat{W}^k \hat{H}_k = \sum_{k=1}^{r} W^*k H^*_k = W^* H^*,
\]

and thus \(F(W^*, H^*) = F(\hat{W}, \hat{H})\), i.e., these two pairs of matrices have the same value. Furthermore, note that

\[
\left\|\hat{W}^k\right\|_1 + \left\|\hat{H}_k\right\|_1 = 2 \left(\left\|\hat{W}^k\right\|_1 \left\|\hat{H}_k\right\|_1\right)^{\frac{1}{2}} = 2 \left(\sum_{i,j} W^*_{ik} H^*_kj\right)^{\frac{1}{2}}
\]

\[
= 2 \left[\sum_{i,j} W^*_{ik} H^*_kj^2\right]^{\frac{1}{4}}
\]

\[
\leq 2 \left[\sum_{i,j} nW^*_{ik} H^*_kj^2\right]^{\frac{1}{4}}
\]

\[
\leq 2(nm)^{\frac{1}{4}} \|W^* H^*\|_F^{\frac{1}{4}} \leq 2(nm)^{\frac{1}{4}} \|V\|_F^{\frac{1}{4}} = C.
\]

Lastly, consider the parametrized family of matrix pairs \((t\hat{W}, t^\frac{1}{4}\hat{H})\) and increase \(t\) until

\[
t \left(\sum_{i,k} \hat{W}_{ik}\right) + \frac{1}{t} \left(\sum_{k,j} \hat{H}_{kj}\right) = C.
\]

This leads to a pair of matrices that are FOSP of (S-NMF).

4 Proof of Lemma 2

Let \((W^s, H^s)\) be a SOSP of the problem (S-NMF) with \(c \neq 0\). We will arrive at a contradiction by showing the existence of a pair of matrices \((W^s, H^s)\) satisfying:

\[
\frac{\partial F(W^s, H^s)}{\partial W^s_{ik}} > c \implies W^s_{ik} = 0, \tag{8}
\]

\[
\frac{\partial F(W^s, H^s)}{\partial H^s_{kj}} > c \implies H^s_{kj} = 0. \tag{9}
\]
\[ \sum_{i,k} W_{ik}^s + \sum_{k,j} H_{kj}^s = 0, \quad (10) \]
\[ s^\top \nabla^2 F(W^*, H^*) s < 0, \]

where we set \( s^\top = (\text{vec}(W^s)^\top, \text{vec}(H^s)^\top) \). We start with a technical claim that will be used up next.

**Lemma 4.** Let \((W^*, H^*)\) be a FOSP for \((S-NMF)\), for some constant \(c \neq 0\). Then for all \(k \in \{1, \ldots, r\}\), we have
\[ \sum_{i=1}^n W_{ik}^* = \sum_{j=1}^m H_{kj}^*. \]

**Proof.** Direct calculation reveals that:
\[
\begin{align*}
    c \sum_{i=1}^n W_{ik}^* &= \sum_{i : W_{ik}^* > 0} W_{ik}^* \cdot c \\
    &= \sum_{i : W_{ik}^* > 0} W_{ik}^* \cdot \frac{\partial F(W^*, H^*)}{\partial W_{ik}} \\
    &= \sum_{i=1}^n W_{ik}^* \left[ -2 \sum_{j=1}^m \left( V_{ij} - \sum_{\ell=1}^r W_{i\ell}^* H_{\ell j}^* \right) H_{kj}^* \right] \\
    &= \sum_{j=1}^m H_{kj}^* \left[ -2 \sum_{i=1}^n \left( V_{ij} - \sum_{\ell=1}^r W_{i\ell}^* H_{\ell j}^* \right) W_{ik}^* \right] \\
    &= c \sum_{j=1}^m H_{kj}^*. \\
\end{align*}
\]

We are now ready to describe the construction of the matrices \((W_s, H_s)\) satisfying (8)-(11). Setting
\[ k = \arg \max_{1 \leq \ell \leq r} \left( \sum_{i=1}^n W_{i\ell}^* + \sum_{j=1}^m H_{\ell j}^* \right), \]
it follows immediately by Lemma 4 that
\[ \|W^{*k}\|_1 = \|H_k^*\|_1 \geq C/2r. \quad (12) \]

The matrices \(W^s, H^s\) are defined as follows: \( W_{ik}^s = W_{ik}^* \), \( H_{kj}^s = -H_{kj}^* \), while \( W_{i\ell}^s = H_{\ell j}^* = 0 \), i.e., the \(k\)-th column of \(W^s\) coincides with the \(k\)-th column of \(W^*\) and all other entries are zero. It is immediate from the definition that Conditions (8)-(9) are satisfied, since \( \frac{\partial F(W^*, H^*)}{\partial W_{ki}} > c \) implies
\( W^*_{ik} = 0 \) (by Condition (3)) and thus \( W^s_{ik} = 0 \), by the definition of \( W^s \) (and analogously for \( H^*_k \)). Moreover, Condition (10) is satisfied since

\[
\sum_{i=1}^{n} \sum_{k=1}^{r} W^s_{ik} + \sum_{j=1}^{m} \sum_{k=1}^{r} H^s_{kj} = \sum_{i=1}^{n} W^*_{ik} - \sum_{j=1}^{m} H^*_kj = 0,
\]

where the last equality follows from Lemma 4.

It remains to verify Condition (11). By Lemma 3, we have that

\[
s^\top \nabla^2 F(W^*, H^*) s = (\text{vec}(W^s)^\top, \text{vec}(H^s)^\top) \cdot \nabla^2 F(W^*, H^*) \cdot (\text{vec}(W^s), \text{vec}(H^s))
\]

\[
= (\text{vec}(W^s)^\top, \text{vec}(H^s)^\top) \cdot \begin{pmatrix}
0 & -\nabla W^s F(W^*, H^*) \\
0 & \nabla H^s F(W^*, H^*)
\end{pmatrix}
\]

\[
= \sum_{i=1}^{n} \left( -\frac{\partial F(W^*, H^*)}{\partial W_{ik}} \right) W^s_{ik} + \sum_{i=1}^{n} \frac{\partial F(W^*, H^*)}{\partial H_{kj}} H^s_{kj}
\]

\[
= \sum_{i=1}^{n} \left( -\frac{\partial F(W^*, H^*)}{\partial W_{ik}} \right) W^*_{ik} + \sum_{i=1}^{n} \frac{\partial F(W^*, H^*)}{\partial H_{kj}} (-H^*_{kj})
\]

\[
= 2 \sum_{i=1}^{n} \sum_{j=1}^{m} V_{ij} W^s_{ik} H^s_{kj} - 2 \sum_{i=1}^{n} \sum_{j=1}^{m} W^s_{ik} H^s_{kj} \sum_{\ell=1}^{r} W^*_{ik} H^*_{kj}
\]

\[
\leq 2 \sum_{i=1}^{n} \sum_{j=1}^{m} V_{ij} W^s_{ik} H^s_{kj} - 2 \sum_{i=1}^{n} \sum_{j=1}^{m} W^s_{ik}^2 H^s_{kj}^2
\]

\[
\leq 2 \|V\|_F \|W^s H^s\|_F - 2 \left\|W^s H^s\right\|_F^2
\]

where the first inequality follows from the fact that all the entries \( W^s_{ij}, H^s_{kj} \) are positive and the second from the Cauchy-Schwarz inequality. In order to satisfy Condition (11), it remains to show that \( \|V\|_F - \|W^s H^s\|_F < 0 \). Indeed,

\[
\left\|W^s H^s\right\|_F^2 = \sum_{i=1}^{n} \sum_{j=1}^{m} W^s_{ik}^2 H^s_{kj}^2
\]

\[
\geq \frac{1}{nm} \left( \sum_{i=1}^{n} \sum_{j=1}^{m} W^s_{ik} H^s_{kj} \right)^2
\]

\[
= \frac{1}{nm} \left( \sum_{i=1}^{n} W^s_{ik} \right)^2 \left( \sum_{j=1}^{m} H^s_{kj} \right)^2
\]

\[
\geq \frac{1}{16nm} \left( \|W^s\|_1 \right)^4,
\]

where the last inequality follows by Claim 4. Combining the above with (12) we arrive at,

\[
\left\|W^s H^s\right\|_F \geq \frac{C^2}{4r^2 \sqrt{nm}} > \|V\|_F,
\]

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where we used that $C > 2r(nm)^{\frac{1}{2}}\|V\|_F$.

5 Proof of Theorem 2

Let $(W^*, H^*)$ be a second-order stationary point of the problem (S-NMF) which is not a second-order stationary point of the unconstrained problem (NMF). Since $(W^*, H^*)$ is a SOSP of (S-NMF), Lemma 2 implies that $c = 0$.

As in the proof of Lemma 2, we will arrive at a contradiction by identifying a non-zero pair of matrices $(W_s, H_s)$ that satisfy the following 4 conditions:

\begin{align*}
\frac{\partial F(W^*, H^*)}{\partial W_{ik}} > 0 & \implies W_{ik}^s = 0, \quad (14) \\
\frac{\partial F(W^*, H^*)}{\partial H_{kj}} > 0 & \implies H_{kj}^s = 0, \quad (15) \\
\sum_{i,k} W_{ik}^s + \sum_{k,j} H_{kj}^s = 0, \quad (16) \\
s^\top \nabla^2 F(W^*, H^*) s < 0, \quad (17)
\end{align*}

where we set $s^\top = (\text{vec}(W^s)^\top, \text{vec}(H^s)^\top)$.

As $(W^*, H^*)$ is not a SOSP of (NMF), there exist a pair of matrices $(\hat{W}, \hat{H})$ satisfying conditions (14), (15) and (17). In the construction of the pair $(W^*, H^*)$, we will use the pair $(\hat{W}, \hat{H})$ to construct a new pair $(W_s, H_s)$ that also satisfies (16). We remind that $\hat{W}_{ik} = W_{ik}^*, \hat{H}_{kj} = -H_{kj}^*$ and $\hat{W}_i = \hat{H}_j = 0$. Moreover (0 denotes the zero column vector of appropriate size),

\[
(\text{vec}(\hat{W})^\top, \text{vec}(\hat{H})^\top) \cdot \nabla^2 F(W^*, H^*) = \begin{pmatrix} 0^\top \\ -\nabla_{W^k}^* F(W^*, H^*) \\ \nabla_{H^k}^* F(W^*, H^*) \\ 0^\top \end{pmatrix}.
\]

We are now ready to describe our construction. Consider the following family of matrix pairs:

$$(W^t, H^t) = (\tilde{W}, \tilde{H}) + t(\hat{W}, \hat{H})^1,$$

which we show satisfies Conditions (14), (15) and (17). Indeed, assuming that $\frac{\partial F(W^*, H^*)}{\partial W_{ik}} > 0$, it follows by (14) that $W_{ik}^t = 0$, and furthermore, as $(W^*, H^*)$ is a SOSP for (S-NMF), we also have that $W_{ik}^s = 0$ and thus $W_{ik}^t = 0$. Combining these we get that $W_{ik}^t = 0$, i.e., $(W^t, H^t)$ satisfies (14) for all $t$. Analogously, if $\frac{\partial F(W^*, H^*)}{\partial H_{kj}} > 0$ it follows that $H_{kj}^t = 0$.

Lastly, we show that for all $t \neq 0$, the pair of matrices $(W^t, H^t)$ satisfy (17). To simplify notation let,

- $s_t^\top = (\text{vec}(W^t)^\top, \text{vec}(H^t)^\top)$, respectively $\hat{s}$ for $(\tilde{W}, \tilde{H})$ and $\hat{s}$ for $(\hat{W}, \hat{H})$.

- $\nabla^2 = \nabla^2 F(W^*, H^*)$.

\[\text{(vec(\hat{W})^\top, vec(\hat{H})^\top)} \cdot \nabla^2 F(W^*, H^*) = \begin{pmatrix} 0^\top \\ -\nabla_{W^k}^* F(W^*, H^*) \\ \nabla_{H^k}^* F(W^*, H^*) \\ 0^\top \end{pmatrix}.
\]

\[\text{where we set s^\top = (vec(W^s)^\top, vec(H^s)^\top).}
\]

\[\text{1slightly abusing notation since, W^t up to now means the t-th column}
\]

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Then, we have that
\[ s_t^T \nabla^2 s_t = (s + ts)^T \nabla^2(s + ts) = s^T \nabla^2 s + 2ts^T \nabla^2 s + t^2 s^T \nabla^2 s \]
\[ = (0, -\nabla_{Wk} F(W^*, H^*), 0, \nabla_{Hk} F(W^*, H^*), 0)^T \cdot s \]
\[ + 2t(0, -\nabla_{Wk} F(W^*, H^*), 0, \nabla_{Hk} F(W^*, H^*), 0)^T \cdot s \]
\[ + t^2 s^T \nabla^2 s < 0 \]
where for the second equality we use Lemma 3. The first term is zero since if \( \hat{W}_{ik} \neq 0 \) implies that \( W^*_{ik} \neq 0 \) which implies that \( \frac{\partial F(W^*, H^*)}{\partial W_{ik}} = 0 \) since \( (W^*, H^*) \) is a SOSP (analogously for \( H_{kj} \)). By Conditions (14)-(15), we know that if \( \frac{\partial F(W^*, H^*)}{\partial W_{ik}} > 0 \) then \( \hat{W}_{ik} = 0 \) (analogously for \( H_{kj} \)), meaning that the second term is also zero. Finally, the third term is strictly negative as \( (W, \hat{H}) \) satisfies (17).

We complete the proof of Theorem 2 by noting that for
\[ t = \frac{\sum_{i=1}^{n} \sum_{k=1}^{r} \hat{W}_{ik} + \sum_{k=1}^{r} \sum_{j=1}^{m} \hat{H}_{kj}}{\sum_{i=1}^{n} \sum_{k=1}^{r} \tilde{W}_{ik} + \sum_{k=1}^{r} \sum_{j=1}^{m} \tilde{H}_{kj}} = -\frac{\sum_{i=1}^{n} W^*_{ik} - \sum_{j=1}^{m} H^*_{kj}}{\sum_{i=1}^{n} \sum_{k=1}^{r} \tilde{W}_{ik} + \sum_{k=1}^{r} \sum_{j=1}^{m} \tilde{H}_{kj}}, \]
the remaining Condition (16) is satisfied. An important detail is that \( t \neq 0 \) since \( \sum_{i=1}^{n} W^*_{ik} = \sum_{j=1}^{m} H^*_{kj} \) contradicts with the assumption that \( (W^*, H^*) \) is SOSP (recall the proof of Lemma 2 in Section 4).

6 Examples and Experiments

In this section we present experimental evaluations on the quality of the solutions produced by the Multiplicative Weight Update algorithm (Algorithm 1), which indicate convergence to the global minimizers. More precisely, for several values of the parameters \( n \) and \( r \), we generated random \( n \times n \) matrices with entries in \([0, 1]\) and rank \( r \) and we checked the quality of the solutions \( W_{n \times r}, H_{n \times r} \) produced by MWU. This was done so as to ensure that the global minimum of the respective NMF problem is 0, which served as a benchmark on the quality of the solutions produced by MWU. For all the conducted experiments MWU was able to find a solution with value arbitrarily close to 0 meaning that it always converged to the right factorization. Figure 1 illustrates the number of iterations needed MWU to converge to solutions with error smaller than 1% of the initial error, for various values of \( n, r \).

An important differentiation of the Multiplicative Weight Update depicted in Algorithm 1 with the previous multiplicative weight update and gradient based approaches, is its concurrent way of updating the entries of \( W \) and \( H \). Both the matrices \( W^{t+1} \) and \( H^{t+1} \) are updated by using only the values of \( W^t \) and \( H^t \). We remark that that concurrency in the updating step is very desirable, since it permits more efficient implementations in parallel computing environments. To the best of our knowledge, Algorithm 1 is the first iterative method for non-negative matrix factorization that converges while performing its updates in a concurrent way. In all the previous gradient based approaches (both in multiplicative weight algorithms and in alternating least squares) the convergence properties heavily rely on the fact that the entries of \( W \) and \( H \) are updating in an
alternating way, while their concurrent counterparts may fail to converge. In Example 1 we present such a case for the Lee-Seung algorithm in which the original version of the algorithm converges, while the concurrent version fails to converge.

**Example 1.** Consider the matrices $V = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $W^0 = H^0 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ initialize the concurrent version of Lee-Seung algorithm i.e. $W_{ik}^{t+1} = W_{ik}^t \frac{(W^T V)_{ik}}{(W^T W_t H_t)_{ik}}$ and $H_{kj}^{t+1} = H_{kj}^t \frac{(V H_t^T)_{kj}}{(W_t H_t H_t^T)_{kj}}$. Then $(W^t, H^t)$ oscillates.

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Figure 2: The error of the concurrent Lee-Seung algorithm versus the error of the original algorithm in the NMF instance described in Example 1.

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