Supporting document for the paper
“Stability analysis of multiplicative update algorithms
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Document de support pour l’article
« Analyse de la stabilité des règles de mises à jour
multiplicatives et application à la factorisation en
matrices positives »

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Document de support pour l’article "Analyse de la stabilité des règles de mises à jour multiplicatives et application à la factorisation en matrices positives"

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Abstract

Multiplicative update algorithms have encountered a great success to solve optimization problems with non-negativity constraints, such as the famous non-negative matrix factorization (NMF) and its many variants. However, despite several years of research on the topic, the understanding of their convergence properties is still to be improved. In reference [1], we show that Lyapunov’s stability theory provides a very enlightening viewpoint on the problem. We prove the exponential or asymptotic stability of the solutions to general optimization problems with non-negative constraints, including the particular case of supervised NMF, and finally study the more difficult case of unsupervised NMF. The theoretical results presented in the paper are confirmed by numerical simulations involving both supervised and unsupervised NMF, and the convergence speed of NMF multiplicative updates is investigated. In this supporting document, we present the proofs of some theoretical results presented in [1]. This document, written as a sequel of [1], is not intended to be read separately.

Index Terms

Optimization methods, non-negative matrix factorization, multiplicative update algorithms, convergence of numerical methods, stability, Lyapunov methods.

Résumé

Les règles de mises à jour multiplicatives ont connu un grand succès pour résoudre des problèmes d’optimisation avec contraintes de positivité, tels que la célèbre factorisation en matrices positives (NMF) et ses nombreuses variantes. Néanmoins, malgré plusieurs années de recherche sur le sujet, la compréhension de leurs propriétés de convergence demeure imparfaite. Dans la référence [1], nous prouvons que la théorie de la stabilité de Lyapunov fournit un point de vue très instructif sur le problème. Nous prouvons la stabilité exponentielle ou asymptotique des solutions de problèmes généraux d’optimisation avec contraintes de positivité, incluant le cas particulier de la NMF supervisée, et nous étudions finalement le cas difficile de la NMF non supervisée. Les résultats théoriques présentés dans cet article sont validés par des simulations numériques mettant en œuvre les deux types de NMF, et la vitesse de convergence des mises à jour multiplicatives est examinée. Dans ce document de support, nous présentons les preuves de certains résultats théoriques présentés dans [1]. Ce document, faisant suite à [1], n’est pas destiné à être lu séparément.

Mots clés

Méthodes d’optimisation, factorisation en matrices positives, algorithmes de mises à jour multiplicatives, convergence des méthodes numériques, stabilité, méthodes de Lyapunov.

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INTRODUCTION

In the following developments, we use the notation introduced in sections III and IV of reference [1]. This supporting document is organized as follows: section VII is devoted to the proof of Lemma 13 in section IV-A of reference [1], and section VIII is devoted to the proof of Proposition 16.

We begin with a key result in linear algebra:

**Theorem 18.** Let $M$ and $N$ be two real square matrices of same dimension. Suppose that $M$ is non-singular, $M^T + N$ is positive definite, and $M - N$ is positive semidefinite. Then any vector in the kernel of $M - N$ is an eigenvector of matrix $M^{-1}N$, whose eigenvalue is 1. Moreover, all other eigenvalues of $M^{-1}N$ have modulus lower than 1.

*Proof:* First note that $M - N = (M + M^T) - (M^T + N)$, which proves that this matrix is symmetric. Moreover, any vector in its kernel is obviously an eigenvector of matrix $M^{-1}N$, whose eigenvalue is 1. Then let $x$ be a complex vector such that $(M - N)x \neq 0$, normalized so that $x^H(M - N)x = 1$. Straightforward calculations show that
\[
(M^{-1}N x)^H (M - N)(M^{-1}N x) = 1 - y^H (M^T + N)y
\]
where $y = M^{-1}(M - N)x \neq 0$. As $M^T + N$ is positive definite, the right member of equation (41) is lower than 1. If moreover $x$ is an eigenvector of matrix $M^{-1}N$ associated to an eigenvalue $\lambda \neq 1$, then the left member of this equation is equal to $|\lambda|^2$, which proves that $|\lambda| < 1$. 

VII. PRELIMINARY RESULTS

A. Gradient and Hessian matrix of the objective function

In this section, we provide closed form expressions of the gradient and the Hessian matrix of the objective function $J$ defined in equation (17). Following Notation 2, we define for all $f \in \{1 \ldots F\}$ and $t \in \{1 \ldots T\}$ the vectors $w_f = [w_f1, \ldots, w_fK]^T$ and $h_t = [h_t1, \ldots, h_tK]^T$, so that we can write $w^T = [w^T_1, \ldots, w^T_F]$, $h^T = [h^T_1, \ldots, h^T_T]$, and $x^T = [w^T, h^T]$.

1) First and Second order partial derivatives: Assume that divergence $d$ in equation (1) is twice continuously differentiable. Then for all $f \in \{1 \ldots F\}$ and $t \in \{1 \ldots T\}$, the first order partial derivatives of the objective function $J$ defined in equation (17) are
\[
\nabla_{w_f} J(x) = \sum_{t=1}^T d'(v_{ft}|\hat{v}_{ft}) h_t
\]
\[
\nabla_{h_t} J(x) = \sum_{f=1}^F d'(v_{ft}|\hat{v}_{ft}) w_f
\]
where $\hat{v}_{ft}$ was defined in equation (5). The second order partial derivatives are obtained by differentiating these expressions. First note that if $f_1 \neq f_2$, $\nabla^2_{w_{f_1}w_{f_2}} J(x) = 0$, and if $t_1 \neq t_2$, $\nabla^2_{h_{t_1}h_{t_2}} J(x) = 0$, thus matrices $\nabla^2_{w_{f}w_{f}} J(x)$ and $\nabla^2_{h_{t}h_{t}} J(x)$ are block-diagonal. Moreover,
\[
\nabla^2_{w_{f}w_{f}} J(x) = \sum_{t=1}^T d''(v_{ft}|\hat{v}_{ft}) h_t h^T_t
\]
\[
\nabla^2_{h_{t}h_{t}} J(x) = \sum_{f=1}^F d''(v_{ft}|\hat{v}_{ft}) w_f w^T_f
\]
\[
\nabla^2_{h_{t}w_{f}} J(x) = d''(v_{ft}|\hat{v}_{ft}) w_f h^T_t + d'(v_{ft}|\hat{v}_{ft}) I_K
\]
where $I_K$ denotes the $K \times K$ identity matrix.

It follows that if the divergence $d$ is convex (i.e. $d'' \geq 0$), then matrices $\nabla^2_{w_{f}w_{f}} J(x)$ and $\nabla^2_{h_{t}h_{t}} J(x)$ are both positive semi-definite and non-negative (they are called doubly non-negative). In particular, the positive semi-definite property confirms that the objective function $J$ is convex w.r.t. $w$ ($h$ being fixed), and also convex w.r.t. $h$ ($w$ being fixed).
2) Case of the $\beta$-divergence: From now on, we focus on the $\beta$-divergence defined in equation (2). Let $\beta \in \mathbb{R}$, the first and second order derivatives of $d_\beta(x|y)$ w.r.t. $y$ are

$$
 d'_\beta(x|y) = y^{\beta-1} \left( 1 - \frac{x}{y} \right)
$$
$$
 d''_\beta(x|y) = y^{\beta-2} \left( (\beta - 1) + (2 - \beta) \frac{x}{y} \right)
$$

The last equality shows that the $\beta$-divergence is convex if and only if $1 \leq \beta \leq 2$. It follows that in this case, matrices $\nabla^2_{w_w} J(x)$ and $\nabla^2_{h_h} J(x)$ are doubly non-negative.

B. Notation

Using the results of section VII-A, the gradients of the objective function w.r.t. $w$ and $h$ can be written as the difference of two non-negative terms:

$$
\begin{align*}
\nabla_{w} J(x) &= p^{w}(x) - m^{w}(x) \\
\nabla_{h} J(x) &= p^{h}(x) - m^{h}(x)
\end{align*}
$$

(42)

where $p^{w}(x) = [p^{w_1}(x); \ldots; p^{w_F}(x)]$, vectors $m^{w}(x)$, $p^{h}(x)$, and $m^{h}(x)$ being formed in a similar way, and

$$
\begin{align*}
p^{w_f}(x) &= \sum_{t=1}^{T} \hat{v}_{ft}^{\beta-1} h_t \\
m^{w_f}(x) &= \sum_{t=1}^{T} \hat{v}_{ft}^{\beta-1} v_{ft} h_t \\
p^{h_f}(x) &= \sum_{f=1}^{F} \hat{v}_{ft}^{\beta-1} w_f \\
m^{h_f}(x) &= \sum_{f=1}^{F} \hat{v}_{ft}^{\beta-1} v_{ft} w_f
\end{align*}
$$

Note that these expressions correspond to those already provided in equations (5) and (32) (see Notation 2). In the next section, we will use the following result:

**Lemma 19.** Let $J$ be the objective function defined in equation (17). Then using Notation 2, $\forall \beta \in \mathbb{R}$, $\forall x \in \mathbb{R}^{K(F+N)}$,

$$
\begin{align*}
\nabla_{h} J(x) \quad h &= (2 - \beta) \nabla_{h} J(x), \\
\nabla_{w} J(x) \quad w &= -(\beta - 1) \nabla_{h} J(x).
\end{align*}
$$

Proof: Equation (43) is proved by noting that matrix $\nabla^2_{h} J(x)$ is block-diagonal (as mentioned in section VII-A1), and that $\forall t \in \{1 \ldots T\}$,

$$
\nabla^{2}_{h,h} J(x) h_t = \left( \sum_{f=1}^{F} \hat{v}_{ft}^{\beta-2} \left( (\beta - 1) + (2 - \beta) \frac{v_{ft}}{v_{ft}} \right) w_f w_f^T \right) h_t
$$

$$
= \sum_{f=1}^{F} \hat{v}_{ft}^{\beta-1} w_f - (2 - \beta) \sum_{f=1}^{F} \hat{v}_{ft}^{\beta-1} (1 - \frac{v_{ft}}{v_{ft}}) w_f
$$

$$
= p^{h_f}(x) - (2 - \beta) \nabla_{h} J(x)
$$

Equation (44) is proved by noting that $\forall t \in \{1 \ldots T\}$ and $\forall f \in \{1 \ldots F\}$,

$$
\nabla^{2}_{h,w} J(x) w_f = \hat{v}_{ft}^{\beta-1} \left( (\beta - 1) + (2 - \beta) \frac{v_{ft}}{v_{ft}} \right) w_f + \hat{v}_{ft}^{\beta-1} (1 - \frac{v_{ft}}{v_{ft}}) w_f
$$

thus

$$
\sum_{f=1}^{F} \nabla^{2}_{h,w} J(x) w_f = \sum_{f=1}^{F} \hat{v}_{ft}^{\beta-1} w_f + (\beta - 1) \sum_{f=1}^{F} \hat{v}_{ft}^{\beta-1} (1 - \frac{v_{ft}}{v_{ft}}) w_f
$$

$$
= p^{h_f}(x) + (\beta - 1) \nabla_{h} J(x)
$$

\[\square\]
C. Upper bound for the exponent step size $\eta$

We can now prove Lemma 13.

**Proof of Lemma 13.** Lemma 20 below shows that matrix $P_h(x)$ has an eigenvalue equal to 1 (see equation (46)). Thus $\|P_h(x)\|_2 \geq 1$. This proves that $\eta^*_h \leq 2$. If moreover $\beta \in [1, 2]$, lemma 22 additionally shows that 1 is the greatest eigenvalue of matrix $P_h(x)$, thus $\|P_h(x)\|_2 = 1$. This finally proves that $\eta^*_h = 2$. ■

**Lemma 20.** Given a constant vector $w$, let $h$ be a local minimum of the NMF objective function $h \mapsto J(w, h)$ defined in equation (17). Function $h \mapsto J(w, h)$ satisfies Assumption 7 and we assume that $h$ satisfies Assumption 2.

Let decompose the matrix $P(x)$ defined in equation (29) into four sub-blocks:

$$P(x) = \begin{bmatrix} P^w(x) & P^{wh}(x) \\ P^{hw}(x) & P^h(x) \end{bmatrix}$$

(where matrices $P^h(x)$ and $P^w(x)$ were already defined in equations (21) and (24)). Then

$$P^h(x) D^h(x) p^h(x) = D^h(x) p^h(x)$$

$$P^{hw}(x) D^w(x) p^w(x) = D^h(x) p^h(x)$$

**Proof:** Let prove equation (44). Since $h$ is a local minimum of the objective function $J$, all non-zero coefficients of vector $\nabla_h J(x)$ correspond to zero coefficients of vector $h$, thus $D^h(x) \nabla_h J(x) = 0$. Consequently, equation (43) yields $D^h(x) \nabla_{hh}^2 J(x) h = D^h(x) p^h(x)$, which is equivalent to $P^h(x) D^h(x) p^h(x) = D^h(x) p^h(x)$.

Then let prove equation (47). Since $D^h(x) \nabla_h J(x) = 0$, equation (44) yields $D^h(x) \nabla_{hw}^2 J(x) w = D^h(x) p^h(x)$, which is equivalent to $P^{hw}(x) D^w(x) p^w(x) = D^h(x) p^h(x)$. ■

**Lemma 21.** Given a constant vector $h$, let $w$ be a local minimum of the NMF objective function $w \mapsto J(w, h)$ defined in equation (17). Function $w \mapsto J(w, h)$ satisfies Assumption 7 and we assume that $w$ satisfies Assumption 2.

Let decompose the matrix $P(x)$ defined in equation (29) into four sub-blocks, as in equation (45). Then

$$P^w(x) D^w(x) p^w(x) = D^w(x) p^w(x)$$

$$P^{wh}(x) D^h(x) p^h(x) = D^w(x) p^w(x)$$

**Lemma 22.** Given a constant vector $w$, let $h$ be a local minimum of the NMF objective function $h \mapsto J(w, h)$ defined in equation (17). Function $h \mapsto J(w, h)$ satisfies Assumption 7 and we assume that $h$ satisfies Assumption 2. If $\beta \in [1, 2]$ then all the eigenvalues of the positive semidefinite matrix $P^h(x)$ are lower than or equal to 1.

**Proof:** First, note that the eigenvalues of matrix $P^h(x)$ are the same as those of matrix $M^{-1} N$, where $M = \text{diag}(p^h(x))$, and $N = \text{diag}(\sqrt{h}) \nabla_{hh}^2 J(x) \text{diag}(\sqrt{h})$. Obviously, $M^2 + N$ is positive definite. Let us prove by contradiction that $M - N$ is positive semidefinite. Thus assume that $M - N$ has an eigenvalue $\lambda < 0$. Then matrix $\text{diag}(p^h(x)) - \nabla_{hh}^2 J(x) \text{diag}(h) - \lambda I$ is singular. However, since $h$ is a local minimum of the objective function $J$, all coefficients of vector $\nabla_h J(x)$ are non-negative, thus equation (43) proves that all coefficients of vector $p^h(x) - \nabla_{hh}^2 J(x) h$ are non-negative. Besides, since $\beta \in [1, 2]$, $d_\beta$ is convex, thus matrix $\nabla_{hh}^2 J(x)$ is non-negative. This proves that matrix $\text{diag}(p^h(x)) - \nabla_{hh}^2 J(x) \text{diag}(h) - \lambda I$ is diagonally dominant (the difference between a diagonal coefficient and the sum of the absolute values of the other coefficients in the same row is greater than or equal to $-\lambda > 0$). Consequently, this matrix is non-singular, which contradicts the previous assertion. As a conclusion, all eigenvalues of $M - N$ are non-negative, thus this matrix is positive semidefinite. Lemma 22 is finally proved by applying Theorem 18 to matrices $M$ and $N$. ■
VIII. LYAPUNOV’S FIRST METHOD

A. Expression of the Jacobian matrix

Straightforward calculations show that the Jacobian matrix of function $\phi$ defined in equation (27) satisfies

$$\nabla \phi^T = \begin{bmatrix} \nabla_w \phi^{wT} & 0 \\ \nabla_h \phi^{wT} & I \\ \nabla_w \phi^{hT} & \nabla_h \phi^{hT} \end{bmatrix}$$

where

$$\begin{align*}
\nabla_w \phi^{wT} &= \Lambda_w \eta + \eta \nabla_w m^{wT} \text{diag}(\phi^w / m^w) \\
\nabla_h \phi^{hT} &= \Lambda_h \eta + \eta \nabla_h m^{hT} \text{diag}(\phi^h / m^h) \\
\nabla_h \phi^{wT} &= \eta \nabla_h m^{wT} \text{diag}(\phi^w / m^w) \\
\nabla_w \phi^{hT} &= \eta \nabla_w m^{hT} \text{diag}(\phi^h / m^h)
\end{align*}$$

(50)

By differentiating equation (42), it can be noticed that if $x$ is a fixed point of $\phi$ (such that $\phi^w(w, h) = w$ and $\phi^h(w, h) = h$), these expressions can be written in a simpler form:

$$\begin{align*}
\nabla_w \phi^{wT}(x) &= \Lambda_w(x) \eta - \eta \nabla_{ww} J(x) D^w(x)^2 \\
\nabla_h \phi^{hT}(x) &= \Lambda_h(x) \eta - \eta \nabla_{hh} J(x) D^h(x)^2 \\
\nabla_h \phi^{wT}(x) &= -\eta \nabla_{hw} J(x) D^w(x)^2 \\
\nabla_w \phi^{hT}(x) &= -\eta \nabla_{wh} J(x) D^h(x)^2
\end{align*}$$

(51-54)

Substituting these equations into (50), we obtain

$$\nabla \phi^T(x) = \Lambda(x) \eta - \eta \begin{bmatrix} \nabla_{ww} J(x) & \Lambda_w(x) \eta \nabla_{wh} J(x) \\ \nabla_{hh} J(x) & \nabla_{hh} J(x) \end{bmatrix} D(x)^2 + \eta^2 \nabla_{xx} J(x) D(x)^2 + \begin{bmatrix} \nabla_{ww} J(x) \end{bmatrix} D(x)^2$$

(55)

B. Eigenvalues of the Jacobian matrix

Using the expression of the Jacobian matrix $\nabla \phi^T(x)$ provided in equation (55), we can now prove Proposition 16.

Proof of Proposition 16. Lemma 5 proves that any local minimum $x$ of the objective function $J$ is a fixed point of $\phi$. Let now have a look at the eigenvalues of matrix $\nabla \phi^T(x)$:

1) For all $i$ such that $x_i = 0$, let $u_i$ be the $i$th column of the identity matrix. Then $u_i$ is a right eigenvector of $\nabla \phi^T(x)$, associated to the eigenvalue $\lambda_i = \left( \frac{m_i(x)}{p_i(x)} \right)^\eta$. We can conclude that if $\nabla_i J(x) = 0$ or $\eta = 0$, then $\lambda_i = 1$; otherwise $\lambda_i \in [0, 1]$ if $\eta > 0$, and $\lambda_i > 1$ if $\eta < 0$.

2) Let $u$ be a right eigenvector of $\nabla \phi^T(x)$ which does not belong to the subspace spanned by the previous ones, associated to an eigenvalue $\lambda$. Left multiplying equation (55) by $D(x)$ and right multiplying it by $u$ yields

$$\begin{align*}
\lambda D(x) u &= D(x) u - \eta D(x) \nabla_{xx} J(x) D(x)^2 u + \eta^2 D(x) \nabla_{xx} J(x) D(x)^2 u + \begin{bmatrix} \nabla_{ww} J(x) \end{bmatrix} D(x)^2 u \\

\end{align*}$$

(56)

Let $v = D(x) u$, and consider the decomposition of matrix $P(x)$ in equation (48). Then equation (56) yields $J(\eta) v = \lambda v$, where

$$J(\eta) = I - \eta P(x) + \eta^2 P(x) \begin{bmatrix} 0 & P^{wh}(x) \\ 0 & 0 \end{bmatrix}.$$
However vector \( \nu \) is non-zero (otherwise \( \nu \) would belong to the space spanned by the previous set of eigenvectors). Therefore \( \nu \) is an eigenvector of matrix \( J(\eta) \), associated to the eigenvalue \( \lambda \). Since for all \( i \) such that \( x_i = 0, v_i = 0 \), \( \nu^*_i \) is also an eigenvector of matrix \( [J(\eta)]*_i \), associated to the same eigenvalue \( \lambda \). As a conclusion, since they have the same cardinality, the set of eigenvalues of the Jacobian matrix \( \nabla \phi^T(x) \) which were not listed in 1) is equal to the set of eigenvalues of matrix \( [J(\eta)]*_i \).

Finally, applying Lemma 23 below to matrices \( [P(x)]*_i \) and \( [J(\eta)]*_i \), we prove that any vector in the kernel of \( [P(x)]*_i \) is a left eigenvector of matrix \( [J(\eta)]*_i \), whose eigenvalue is 1. If moreover \( \eta \in ]0, \eta^*_x \], where \( \eta^*_x \) was defined in equation 23, then all the other eigenvalues of \( [J(\eta)]*_i \) have modulus lower than 1.

Finally, the total number of eigenvalues equal to 1 (if \( \eta \neq 0 \)) is the number of coefficients \( i \) such that \( x_i = 0 \) and \( \nabla_i J(x) = 0 \), plus the dimension of the kernel of matrix \( [P(x)]*_i \). In other words, it is equal to the dimension of the kernel of matrix \( [P(x)]*_i \). To finish this proof, we make the following remarks:

- Lemmas 20 and 21 can be used to prove that vector \( \eta \) is an eigenvector of \( J(\eta) \), whose eigenvalue is 1. Thus \( \lambda = 1 \) is always an eigenvalue of \( \nabla \phi^T(x) \).
- In the same way, lemmas 20 and 21 can be used to prove that vector \( \eta \) is an eigenvector of \( J(\eta) \), whose eigenvalue is \( \lambda = (1 - \eta)^2 \). Thus if \( \eta \notin [0, 2] \), there is at least one eigenvalue greater than 1.

**Lemma 23.** Let \( P \) be a positive semidefinite matrix, decomposed in four sub-blocks: \( P = \begin{bmatrix} P^w & P^{wh} \\ P^{hw} & P^h \end{bmatrix} \), such that \( P^w \) and \( P^h \) are also positive semidefinite. For any \( \eta \in \mathbb{R} \), define matrix

\[
J(\eta) = I - \eta P + \eta^2 P \begin{bmatrix} 0 & P^{wh} \\ 0 & 0 \end{bmatrix}
\]

where \( I \) denotes the identity matrix. Then any vector in the kernel of \( P \) is a left eigenvector of matrix \( J(\eta) \), whose eigenvalue is 1. If moreover \( \eta \in ]0, \eta^*_x \], where \( \eta^*_x \) is defined in equation 23, then all the other eigenvalues of \( J(\eta) \) have modulus lower than 1.

**Proof:** Let

\[
M = \begin{bmatrix} I & 0 \\ \eta P^{hw} & I \end{bmatrix}, \quad N = M - \eta P = \begin{bmatrix} I - \eta P^w & -\eta P^{wh} \\ 0 & I - \eta P^h \end{bmatrix}
\]

Then \( M \) is non-singular, and its inverse matrix is

\[
M^{-1} = \begin{bmatrix} I & 0 \\ -\eta P^{hw} & I \end{bmatrix}
\]

Consequently,

\[
M^{-1} N = M^{-1} (M - \eta P) = I - \eta \begin{bmatrix} I & 0 \\ -\eta P^{hw} & I \end{bmatrix} P = J(\eta)^T
\]

thus its eigenvalues are those of \( J(\eta) \). Besides,

\[
\begin{align*}
M - N & = \eta P \\
M^T + N & = \begin{bmatrix} 2I - \eta P^w & 0 \\ 0 & 2I - \eta P^h \end{bmatrix}
\end{align*}
\]

According to the definition of \( \eta^*_x \), \( M^T + N \) is positive definite if and only if \( \eta < \eta^*_x \). If moreover \( \eta > 0 \), then \( M - N \) is positive semi-definite, and its kernel is equal to that of \( P \). Lemma 23 is thus proved by applying Theorem 18 to matrices \( M \) and \( N \). 

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