Multiplicative Update for a Class of Constrained Optimization Problems Related to NMF and Its Global Convergence

Norikazu Takahashi
Okayama University, Okayama, 700–8530 Japan
Email: takahashi@cs.okayama-u.ac.jp

Masato Seki
Okayama University, Okayama, 700–8530 Japan
Email: seki@momo.cs.okayama-u.ac.jp

***Abstract*—Multiplicative updates are widely used for nonnegative matrix factorization (NMF) as an efficient computational method. In this paper, we consider a class of constrained optimization problems in which a polynomial function of the product of two matrices is minimized subject to the nonnegativity constraints. These problems are closely related to NMF because the polynomial function covers many error function used for NMF. We first derive a multiplicative update rule for those problems by using the unified method developed by Yang and Oja. We next prove that a modified version of the update rule has the global convergence property in the sense of Zangwill under certain conditions. This result can be applied to many existing multiplicative update rules for NMF to guarantee their global convergence.**

I. Introduction

Nonnegative matrix factorization (NMF) [1], [2] is a technique to decompose a given nonnegative matrix $\boldsymbol{X} \in \mathbb{R}_+^{m\times n}$ into two nonnegative matrices $\boldsymbol{W} = (W_{ik}) \in \mathbb{R}_+^{m\times r}$ and $\boldsymbol{H} = (H_{kj}) \in \mathbb{R}_+^{r\times n}$, where $\mathbb{R}_+$ denotes the set of nonnegative numbers, in such a way that $\boldsymbol{WH}$ is approximately equal to $\boldsymbol{X}$. NMF is usually formulated as an optimization problem of the form:

$$\begin{array}{ll} \text{minimize} & D(\boldsymbol{X} \,\|\, \boldsymbol{WH}) \\ \text{subject to} & \boldsymbol{W} \geq \boldsymbol{0}_{m\times r}, \boldsymbol{H} \geq \boldsymbol{0}_{r\times n} \end{array} \tag{1}$$

where $\boldsymbol{0}_{m\times r}$ ($\boldsymbol{0}_{r\times n}$, resp.) is the $m \times r$ ($r \times n$, resp.) matrix of all zeros and the inequality holds componentwise. The objective function $D(\boldsymbol{X} \,\|\, \boldsymbol{WH})$ represents an error between $\boldsymbol{X}$ and $\boldsymbol{WH}$. Euclidean distance and I-divergence are widely used for the error function but various other divergences can also be used (see Reference [3] for example). Strictly speaking, some of those functions are not defined for all points in the feasible region of (1). Hence, for the sake of convenience, we consider them as extended real-valued functions, that is, we add the value $+\infty$ to their range.

Multiplicative update rules, that were first proposed by Lee and Seung [2], [4] for Euclidean distance and I-divergence, are widely used as a simple and efficient computational method for finding local optimal solutions of (1). The basic idea behind this approach is that the new solution is obtained by minimizing an auxiliary function at the current solution, which is strictly convex. Recently, Yang and Oja [3] extended this idea and developed a unified method for deriving multiplicative update rules for eleven error functions including Euclidean distance and I-divergence.

As is well known, each multiplicative update rule decreases the value of the corresponding error function monotonically. However, this does not mean the convergence of the sequence of solutions. One may easily understood this claim by observing the fact that if $(\boldsymbol{W}^*, \boldsymbol{H}^*)$ is a solution to the equation $\boldsymbol{WH} = \boldsymbol{X}$ then all pairs given by $(c\boldsymbol{W}^*, \frac{1}{c}\boldsymbol{H}^*)$ where c is a positive constant are also solutions. In addition, the multiplicative update rules have a serious drawback that they are not defined for all pairs of nonnegative matrices. To avoid this problem, some authors have proposed to modify the original multiplicative update rules so that all entries of $\boldsymbol{W}$ and $\boldsymbol{H}$ are kept positive [5]–[7]. Furthermore, some authors proved that if this modification is used then the sequence of solutions contains at least one convergent subsequence and the limit of any convergent subsequence is a stationary point of the corresponding optimization problem [5], [8]–[10].

In this paper, we focus our attention on the case where the objective function $D(\boldsymbol{X} \,\|\, \boldsymbol{WH})$, which is denoted as $D(\boldsymbol{W}, \boldsymbol{H})$ for simplicity, is expressed as

$$\begin{aligned} & D(\boldsymbol{W}, \boldsymbol{H}) \\ & = a_1 \left(\sum_{ij} b_{1ij} (\boldsymbol{WH})_{ij}^{c_1} \right)^{d_1} + a_2 \left(\sum_{ij} b_{2ij} (\boldsymbol{WH})_{ij}^{c_2} \right)^{d_2} \end{aligned} \tag{2}$$

where $a_t, c_t, d_t \, (t = 1, 2)$ are nonzero constants, $b_{tij} \, (t = 1, 2;\, i = 1, 2, \ldots, m;\, j = 1, 2, \ldots, n)$ are nonnegative constants. $(\boldsymbol{WH})_{ij}$ is the (i, j)-th entry of the matrix $\boldsymbol{WH} \in \mathbb{R}^{m\times n}$. We should note that many error functions used for NMF can be expressed in the form of (2) if we apply

$$\ln z = \lim_{\mu \to 0+} \frac{z^\mu - 1}{\mu}$$

to logarithmic functions. In fact, nine among eleven error functions considered in [3] are covered by (2) (see Table I for more details). The objective of this paper is to find a set of conditions on the constants under which a multiplicative update rule can be derived by the unified approach of Yang and Oja [3] and a modified multiplicative update rule has the global convergence property mentioned above. By doing so, it is expected that a general sufficient condition directly applicable to many error functions are obtained.

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TABLE I. LIST OF ERROR FUNCTIONS THAT CAN BE EXPRESSED IN THE FORM OF THE OBJECTIVE FUNCTION OF (2) (SEE REFERENCE [3] FOR MORE DETAILS). FOR EACH FUNCTION, THE VALUES OF THE CONSTANTS ARE PRESENTED, WHERE X_{ij} IS THE (i, j)-TH ENTRY OF THE NONNEGATIVE MATRIX $\boldsymbol{X}$ THAT HAS TO BE APPROXIMATED BY $\boldsymbol{WH}$, AND μ IS A SUFFICIENTLY SMALL POSITIVE NUMBER.

Error function	a_1	b_{1ij}	c_1	d_1	a_2	b_{2ij}	c_2	d_2
Euclidean distance	1	1	2	1	-2	X_{ij}	1	1
I-divergence	1	1	1	1	$-\frac{1}{\mu}$	X_{ij}	μ	1
Dual I-divergence	$\frac{1}{\mu}$	$X_{ij}^{-\mu}$	$1+\mu$	1	$-\frac{1+\mu}{\mu}$	1	1	1
Itakura-Saito divergence	$-\frac{1}{\mu}$	X_{ij}^{μ}	$-\mu$	1	1	X_{ij}	-1	1
α-divergence								
1) $\alpha > 0$, $\alpha \neq 1$	$\frac{1}{\alpha}$	1	1	1	$-\frac{1}{\alpha(1-\alpha)}$	X_{ij}^{α}	$1-\alpha$	1
2) $\alpha < 0$	$-\frac{1}{\alpha(1-\alpha)}$	X_{ij}^{α}	$1-\alpha$	1	$\frac{1}{\alpha}$	1	1	1
β-divergence ($\beta \neq 0, -1$)	$\frac{1}{1+\beta}$	1	$1+\beta$	1	$-\frac{1}{\beta}$	X_{ij}	β	1
Kullback-Leibler divergence	$\frac{1}{\mu}$	1	1	μ	$-\frac{1}{\mu}$	X_{ij}	μ	1
γ-divergence ($\gamma \neq 0, -1$)	$\frac{1}{\mu(1+\gamma)}$	1	$1+\gamma$	μ	$-\frac{1}{\mu\gamma}$	X_{ij}	γ	μ
Rényi divergence ($\rho > 0, \rho \neq 1$)	$\frac{1}{\mu}$	1	1	μ	$-\frac{1}{\mu(1-\rho)}$	X_{ij}^{ρ}	$1-\rho$	μ

II. MAIN RESULT

For the t-th term ($t \in \{1, 2\}$) of the right-hand side of (2), we define three functions as

$$f_t(x) = a_t x^{d_t}, g_t(x) = a_t x^{c_t d_t} \text{ and } h_t(x) = a_t d_t x^{c_t}. \quad (3)$$

We also define ϕ_1 and ϕ_2 as

$$\phi_t = \begin{cases} c_t d_t, & \text{if } f_t(x) \text{ and } g_t(x) \text{ are convex,} \\ 1, & \text{if } f_t(x) \text{ is convex and } g_t(x) \text{ is concave,} \\ c_t, & \text{if } f_t(x) \text{ is concave and } h_t(x) \text{ is convex,} \\ 1, & \text{if } f_t(x) \text{ and } h_t(x) \text{ are concave.} \end{cases} \quad (4)$$

Applying the method proposed by Yang and Oja [3] to the objective function (2), we obtain a multiplicative update rule, which is formally described as

$$W_{ik}^{(l+1)} = u_{ik}(\boldsymbol{W}^{(l)}, \boldsymbol{H}^{(l)}), \quad (5)$$

$$H_{kj}^{(l+1)} = v_{kj}(\boldsymbol{W}^{(l+1)}, \boldsymbol{H}^{(l)}) \quad (6)$$

where $(\boldsymbol{W}^{(l)}, \boldsymbol{H}^{(l)})$ is the solution after l iterations, $W_{ik}^{(l)}$ is the (i, k)-th entry of $\boldsymbol{W}^{(l)}$, $H_{kj}^{(l)}$ is the (k, j)-th entry of $\boldsymbol{H}^{(l)}$, and the functions u_{ik} and v_{kj} are defined by

$$u_{ik}(\boldsymbol{W}, \boldsymbol{H}) = W_{ik} \left[-\frac{a_2 c_2 d_2 \left(\sum_{pq} b_{2pq} (\boldsymbol{WH})_{pq}^{c_2} \right)^{d_2 - 1}}{a_1 c_1 d_1 \left(\sum_{pq} b_{1pq} (\boldsymbol{WH})_{pq}^{c_1} \right)^{d_1 - 1}} \times \frac{\sum_q b_{2iq} (\boldsymbol{WH})_{iq}^{c_2 - 1} H_{kq}}{\sum_q b_{1iq} (\boldsymbol{WH})_{iq}^{c_1 - 1} H_{kq}} \right]^{\frac{1}{\phi_1 - \phi_2}} \quad (7)$$

and

$$v_{kj}(\boldsymbol{W}, \boldsymbol{H}) = \widetilde{H}_{kj} \left[-\frac{a_2 c_2 d_2 \left(\sum_{pq} b_{2pq} (\boldsymbol{WH})_{pq}^{c_2} \right)^{d_2 - 1}}{a_1 c_1 d_1 \left(\sum_{pq} b_{1pq} (\boldsymbol{WH})_{pq}^{c_1} \right)^{d_1 - 1}} \times \frac{\sum_p b_{2pj} (\boldsymbol{WH})_{pj}^{c_2 - 1} W_{pk}}{\sum_p b_{1pj} (\boldsymbol{WH})_{pj}^{c_1 - 1} W_{pk}} \right]^{\frac{1}{\phi_1 - \phi_2}}. \quad (8)$$

Note that u_{ik} and v_{kj} are not always well-defined. For example, if $f_1(x) = a_1 x^{d_1}$ is convex, $g_1(x) = a_1 x^{c_1 d_1}$ is concave, and both $f_2(x) = a_2 x^{d_2}$ and $h_2(x) = a_2 d_2 x^{c_2}$ are concave then it follows from (4) that $\phi_1 = \phi_2 = 1$. In the following theorem, we give a sufficient condition for u_{ik} and v_{kj} to be well-defined for all positive matrices $\boldsymbol{W}$ and $\boldsymbol{H}$.

Theorem 1: Suppose that the constants in (2) satisfy the following three conditions:

$$a_1 c_1 d_1 > 0 > a_2 c_2 d_2, \quad (9)$$

$$c_1 d_1 > c_2 d_2, \quad (10)$$

$$b_{1ij} > 0 \text{ for all } i \text{ and } j. \quad (11)$$

Then the functions u_{ik} $(i = 1, 2, \ldots, m; k = 1, 2, \ldots, r)$ and v_{kj} $(k = 1, 2, \ldots, r; j = 1, 2, \ldots, n)$ are well-defined and take nonnegative values for all positive matrices $\boldsymbol{W}$ and $\boldsymbol{H}$.

The proof sketch for Theorem 1 will be given in Section IV.

Note that even though the condition in Thoerem 1 is satisfied, the functions u_{ik} and v_{kj} are not defined for all nonnegative matrices. In order to avoid this problem, we take the same approach as in References [6] and [7], that is, we consider the modified multiplicative update rule:

$$W_{ik}^{(l+1)} = \max\left(\epsilon, u_{ik}(\boldsymbol{W}^{(l)}, \boldsymbol{H}^{(l)})\right), \quad (12)$$

$$H_{kj}^{(l+1)} = \max\left(\epsilon, v_{kj}(\boldsymbol{W}^{(l+1)}, \boldsymbol{H}^{(l)})\right) \quad (13)$$

where ϵ is any positive constant. It is apparent from these equations that every entry of $\boldsymbol{W}^{(l)}$ and $\boldsymbol{H}^{(l)}$ is not less than ϵ for all l. Thus it is natural to consider, instead of (1), the modified optimization problem:

$$\begin{array}{ll} \text{minimize} & D(\boldsymbol{W}, \boldsymbol{H}) \\ \text{subject to} & \boldsymbol{W} \geq \epsilon \mathbf{1}_{m \times r}, \ \boldsymbol{H} \geq \epsilon \mathbf{1}_{r \times n} \end{array} \quad (14)$$

where $\mathbf{1}_{m \times r}$ ($\mathbf{1}_{r \times n}$, resp.) is the $m \times r$ ($r \times n$, resp.) matrix of all ones. In the following, the feasible region and the set of stationary points of (14) are denoted by $\mathcal{F}_\epsilon$ and $\mathcal{S}_\epsilon$, respectively.

The following theorem gives a sufficient condition for the modified multiplicative update rule described by (12) and (13) has the global convergence property.

Theorem 2: Suppose that the constants in (2) satisfy (9), (10), (11) and

$$d_1 \geq 1 \geq d_2. \tag{15}$$

Then for any positive constant ϵ and any initial solution $(\boldsymbol{W}^{(0)}, \boldsymbol{H}^{(0)}) \in \mathcal{F}_\epsilon$ the sequence $\{(\boldsymbol{W}^{(l)}, \boldsymbol{H}^{(l)})\}_{l=0}^{\infty}$ generated by (12) and (13) contains at least one convergent subsequence and the limit of any convergent subsequence belongs to $\mathcal{S}_\epsilon$.

The proof sketch for Theorem 2 will be given in Section V.

Let us see which error functions in Table I satisfy the conditions (9), (10), (11) and (15). It is easy to see that for Euclidean distance, I-divergence, α-divergence with $\alpha > 0$ and $\alpha \neq 1$, and β-divergence, all of the four conditions hold. As for Dual I-divergence, Itakura-Saito divergence and α-divergence with $\alpha < 0$, all of the four conditions hold if $\boldsymbol{X}$ is positive[1]. On the other hand, for the last three error functions, at least one of the four conditions does not hold. In case of Kullback-Leibler divergence, (10) does not hold because $c_1 d_1 = c_2 d_2$. As for γ-divergence and Rényi divergence, (15) does not hold because $d_1 = d_2 = \mu < 1$. The problem of these three error functions were recently pointed out by Seki and Takahashi [11].

III. Derivation of Multiplicative Update Rule

In this section, we derive the multiplicative update rule described by (5)–(8) by applying the method of Yang and Oja [3] to (2). To do that, we first need to construct an auxiliary function [4] of (2). Here, $\bar{D}(\boldsymbol{W}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}})$ is called an auxiliary function of (2) if it satisfies $\bar{D}(\boldsymbol{W}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}}) \geq D(\boldsymbol{W}, \boldsymbol{H})$ for all $(\boldsymbol{W}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}}) \in \mathbb{R}_{++}^{m\times r} \times \mathbb{R}_{++}^{r\times n} \times \mathbb{R}_{++}^{m\times r} \times \mathbb{R}_{++}^{r\times n}$ and $\bar{D}(\boldsymbol{W}, \boldsymbol{H}, \boldsymbol{W}, \boldsymbol{H}) = D(\boldsymbol{W}, \boldsymbol{H})$ for all $(\boldsymbol{W}, \boldsymbol{H}) \in \mathbb{R}_{++}^{m\times r} \times \mathbb{R}_{++}^{r\times n}$ where $\mathbb{R}_{++}$ is the set of all positive real numbers.

Let the t-th term of (2) be denoted by $D_t(\boldsymbol{W}, \boldsymbol{H})$, and let $\bar{D}_t(\boldsymbol{W}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}})$ be any auxiliary function of it. Then it is easily seen that $\bar{D}_1(\boldsymbol{W}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}}) + \bar{D}_2(\boldsymbol{W}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}})$ is an auxiliary function of (2). Using the method of Yang and Oja, we obtain $\bar{D}_t(\boldsymbol{W}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}})$ as follows.

1) If both $f_t(x)$ and $g_t(x)$ are convex in $\mathbb{R}_{++}$ then $\bar{D}_t(\boldsymbol{W}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}})$ is given by

$$a_t \left(\sum_{ij} b_{tij} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{ij}^{c_t} \right)^{d_t - 1} \sum_{ij} b_{tij} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{ij}^{c_t - 1} \times \sum_k (\widetilde{W}_{ik}\widetilde{H}_{kj})^{1 - c_t d_t} W_{ik}^{c_t d_t} H_{kj}^{c_t d_t}.$$

2) If $f_t(x)$ is convex and $g_t(x)$ is concave in $\mathbb{R}_{++}$ then $\bar{D}_t(\boldsymbol{W}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}})$ is given by

$$a_t c_t d_t \left(\sum_{ij} b_{tij} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{ij}^{c_t} \right)^{d_t - 1} \times \sum_{ij} b_{tij} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{ij}^{c_t - 1} (\boldsymbol{W}\boldsymbol{H})_{ij} + \text{constant}. \tag{16}$$

3) If $f_t(x)$ is concave and $h_t(x)$ is convex in $\mathbb{R}_{++}$ then $\bar{D}_t(\boldsymbol{W}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}})$ is given by

$$a_t d_t \left(\sum_{ij} b_{tij} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{ij}^{c_t} \right)^{d_t - 1} \sum_{ij} b_{tij} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{ij}^{c_t - 1} \times \sum_k (\widetilde{W}_{ik}\widetilde{H}_{kj})^{1 - c_t} W_{ik}^{c_t} H_{kj}^{c_t} + \text{constant}.$$

4) If both $f_t(x)$ and $h_t(x)$ are concave in $\mathbb{R}_{++}$ then $\bar{D}_t(\boldsymbol{W}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}})$ is given by (16).

The three types of auxiliary functions shown above can be unified into a single formula as

$$\begin{aligned} &\bar{D}_t(\boldsymbol{W}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}}) \\ &= \frac{a_t c_t d_t}{\phi_t} \left(\sum_{ij} b_{tij} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{ij}^{c_t} \right)^{d_t - 1} \sum_{ij} b_{tij} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{ij}^{c_t - 1} \\ &\times \sum_{ij} b_{tij} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{ij}^{c_t - 1} \sum_k (\widetilde{W}_{ik}\widetilde{H}_{kj})^{1 - \phi_t} (W_{ik} H_{kj})^{\phi_t} \end{aligned} \tag{17}$$

where ϕ_t is defined by (4).

The multiplicative update for W_{ik} is obtained by solving

$$\frac{\partial \bar{D}_1}{\partial W_{ik}}(\boldsymbol{W}, \widetilde{\boldsymbol{H}}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}}) + \frac{\partial \bar{D}_2}{\partial W_{ik}}(\boldsymbol{W}, \widetilde{\boldsymbol{H}}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}}) = 0 \tag{18}$$

for W_{ik}. For $t = 1$ and 2, we have

$$\frac{\partial \bar{D}_t}{\partial W_{ik}}(\boldsymbol{W}, \widetilde{\boldsymbol{H}}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}}) = a_t c_t d_t \left(\sum_{pq} b_{tpq} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{pq}^{c_t} \right)^{d_t - 1} \times \left(\frac{W_{ik}}{\widetilde{W}_{ik}} \right)^{\phi_t} \sum_q b_{tiq} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{iq}^{c_t - 1} \widetilde{H}_{kq}.$$

Hence the solution to (18) is formally expressed as

$$W_{ik} = \widetilde{W}_{ik} \left[-\frac{a_2 c_2 d_2 \left(\sum_{pq} b_{2pq} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{pq}^{c_2} \right)^{d_2 - 1}}{a_1 c_1 d_1 \left(\sum_{pq} b_{1pq} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{pq}^{c_1} \right)^{d_1 - 1}} \times \frac{\sum_q b_{2iq} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{iq}^{c_2 - 1} \widetilde{H}_{kq}}{\sum_q b_{1iq} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{iq}^{c_1 - 1} \widetilde{H}_{kq}} \right]^{\frac{1}{\phi_1 - \phi_2}}. \tag{19}$$

Similarly, the multiplicative update for H_{kj} is obtained by solving

$$\frac{\partial \bar{D}_1}{\partial H_{kj}}(\widetilde{\boldsymbol{W}}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}}) + \frac{\partial \bar{D}_2}{\partial H_{kj}}(\widetilde{\boldsymbol{W}}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}}) = 0 \tag{20}$$

for H_{kj}. For $t = 1$ and 2, we have

$$\frac{\partial \bar{D}_t}{\partial H_{kj}}(\widetilde{\boldsymbol{W}}, \boldsymbol{H}, \widetilde{\boldsymbol{W}}, \widetilde{\boldsymbol{H}}) = a_t c_t d_t \left(\sum_{pq} b_{tpq} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{pq}^{c_t} \right)^{d_t - 1} \times \left(\frac{H_{kj}}{\widetilde{H}_{kj}} \right)^{\phi_t} \sum_p b_{tpj} (\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})_{pj}^{c_t - 1} \widetilde{W}_{pk}.$$

[1] If $\boldsymbol{X}$ is not positive, we only have to replace all zeros in $\boldsymbol{X}$ with ϵ.

Hence the solution to (20) is formally expressed as

$$H_{kj} = \widetilde{H}_{kj}\left[-\frac{a_2c_2d_2\left(\sum_{pq} b_{2pq}(\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})^{c_2}_{pq}\right)^{d_2-1}}{a_1c_1d_1\left(\sum_{pq} b_{1pq}(\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})^{c_1}_{pq}\right)^{d_1-1}} \times\frac{\sum_p b_{2pj}(\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})^{c_2-1}_{pj}\widetilde{W}_{pk}}{\sum_p b_{1pj}(\widetilde{\boldsymbol{W}}\widetilde{\boldsymbol{H}})^{c_1-1}_{pj}\widetilde{W}_{pk}}\right]^{\frac{1}{\phi_1-\phi_2}}. \quad (21)$$

IV. Proof Sketch for Theorem 1

In addition to the three conditions (9)–(11), suppose that $\phi_1 \neq \phi_2$. Then the functions u_{ik} and v_{kj} are well-defined and take nonnegative values for all positive matrices $\boldsymbol{W}$ and $\boldsymbol{H}$. Hence, in order to prove Theorem 1, we only need to show that $\phi_1 \neq \phi_2$ under the three conditions.

Lemma 1: If the constants in (2) satisfy (9) and (10) then $\phi_1 > \phi_2$.

Proof: Under the assumption (9) the following eight statements hold true (the proof is omitted due to the limitation of space).

1) If both $f_1(x) = a_1x^{d_1}$ and $g_1(x) = a_1x^{c_1d_1}$ are convex in $\mathbb{R}_{++}$ then $\phi_1 = c_1d_1 \geq 1$ holds.
2) If $f_1(x)$ is convex and $g_1(x)$ is concave in $\mathbb{R}_{++}$ then $\phi_1 = 1$ and $c_1d_1 < 1$ hold.
3) If $f_1(x)$ is concave and $h_1(x) = a_1d_1x^{c_1}$ is convex in $\mathbb{R}_{++}$ then $c_1 \geq 1$, $d_1 < 1$ and $\phi_1 \geq 1$ hold.
4) If both $f_1(x)$ and $h_1(x)$ are concave in $\mathbb{R}_{++}$ then $\phi_1 = 1$ and $c_1d_1 < 1$ hold.
5) If both $f_2(x) = a_2x^{d_2}$ and $g_2(x) = a_2x^{c_2d_2}$ are convex in $\mathbb{R}_{++}$ then $\phi_2 = c_1d_1 < 1$ holds.
6) If $f_2(x)$ is convex and $g_2(x)$ is concave in $\mathbb{R}_{++}$ then $\phi_2 = 1$ and $c_2d_2 > 1$ hold.
7) If $f_2(x)$ is concave and $h_2(x) = a_2d_2x^{c_2}$ is convex in $\mathbb{R}_{++}$ then $\phi_2 = c_2 \leq 1$ hold.
8) If both $f_2(x)$ and $h_2(x)$ are concave in $\mathbb{R}_{++}$ then $\phi_2 = 1$ and $c_2d_2 > 1$ hold.

From these statements, we easily see that $\phi_1 \geq 1$ and $\phi_2 \leq 1$ hold under the assumption (9). In the following, we show that if $\phi_1 = \phi_2 = 1$ then $c_1d_1 < c_2d_2$ which contradicts (10).

If $\phi_1 = 1$ then there are four possible cases:

1) Both $f_1(x)$ and $g_1(x)$ is convex and $c_1d_1 = 1$,
2) $f_1(x)$ is convex and $g_1(x)$ is concave,
3) Both $f_1(x)$ and $h_1(x)$ is concave,
4) $f_1(x)$ is concave, $h_1(x)$ is convex and $c_1 = 1$.

In the second, third and fourth cases, the inequality $c_1d_1 < 1$ holds from the second, fourth, third statements, respectively, given above. If $\phi_2 = 1$ then there are three possible cases:

1) $f_2(x)$ is convex and $g_2(x)$ is concave,
2) Both $f_2(x)$ and $h_2(x)$ is concave,
3) $f_2(x)$ is concave, $h_2(x)$ is convex and $c_2 = 1$.

In the first and second cases, the inequality $c_2d_2 > 1$ holds from the sixth and eighth statements given above. In the third case, we can prove by contradiction that $c_2d_2 = d_2 > 1$. Suppose that $d_2 < 1$. Then either i) $a_2 > 0$ and $0 < d_2 < 1$ or ii) $a_2 < 0$ and $d_2 < 0$ must hold in order for $f_2(x)$ to be concave. Thus $a_2c_2d_2$ must be always positive. However, this contradicts (9). ■

V. Proof Sketch for Theorem 2

We hereafter express (12) and (13) as

$$\boldsymbol{W}^{(l+1)} = U(\boldsymbol{W}^{(l)}, \boldsymbol{H}^{(l)}),$$
$$\boldsymbol{H}^{(l+1)} = V(\boldsymbol{W}^{(l+1)}, \boldsymbol{H}^{(l)})$$

for simplicity, and define the mapping $A : \mathcal{F}_\epsilon \to \mathcal{F}_\epsilon$ as

$$A(\boldsymbol{W}^{(l)}, \boldsymbol{H}^{(l)}) = (U(\boldsymbol{W}^{(l)}, \boldsymbol{H}^{(l)}), V(U(\boldsymbol{W}^{(l)}, \boldsymbol{H}^{(l)}), \boldsymbol{H}^{(l)})).$$

It follows from Zangwill's global convergence theorem [12] that Theorem 2 is valid if the following three statements hold true under the conditions (9), (10), (11) and (15).

1) All points in the sequence $\{(\boldsymbol{W}^{(l)}, \boldsymbol{H}^{(l)})\}_{l=0}^{\infty}$ belong to a compact set in $\mathcal{F}_\epsilon$.
2) There exists a function $z : \mathcal{F}_\epsilon \to \mathbb{R}$ such that $z(A(\boldsymbol{W}, \boldsymbol{H})) < z(\boldsymbol{W}, \boldsymbol{H})$ if $(\boldsymbol{W}, \boldsymbol{H}) \notin \mathcal{S}_\epsilon$ and $z(A(\boldsymbol{W}, \boldsymbol{H})) \leq z(\boldsymbol{W}, \boldsymbol{H})$ if $(\boldsymbol{W}, \boldsymbol{H}) \in \mathcal{S}_\epsilon$.
3) The mapping A is continuous in $\mathcal{F}_\epsilon \setminus \mathcal{S}_\epsilon$.

The second statement can be proved in a similar way as in [9]. Let us next consider the third statement. If the constants in (2) satisfy (9), (10) and (11) then u_{ik} and v_{kj} are continuous in $\mathcal{F}_\epsilon$. Also, for any positive constant ϵ, the function $\max(\epsilon, \cdot)$ is continuous in $\mathcal{F}_\epsilon$. Therefore, the right-hand side of (12) is continuous in $\mathcal{F}_\epsilon$ because it is the composition of u_{ik} and $\max(\epsilon, \cdot)$, and the right-hand side of (13) is continuous in $\mathcal{F}_\epsilon$ because it is the composition of v_{kj} and $\max(\epsilon, \cdot)$.

To prove that the first statement holds true, we make use of the following lemma.

Lemma 2 (Katayama et al. [13]): Let ϵ be any positive constant. If a mapping $f : [\epsilon, \infty) \to \mathbb{R}$ satisfies

$$\forall x \geq \epsilon, \quad f(x) \leq cx^\nu$$

for some $c > 0$ and $\nu < 1$ then for any initial value $x^{(0)} \geq \epsilon$ the sequence $\{x^{(l)}\}_{l=0}^{\infty}$ generated by

$$x^{(l+1)} = \max\left(\epsilon, f(x^{(l)})\right)$$

is contained in a closed and bounded set.

By using this lemma, we obtain the following result.

Lemma 3: Let ϵ be any positive constant. If the constants in (2) satisfy (9), (10), (11) and (15) then for any initial solution $(\boldsymbol{W}^{(0)}, \boldsymbol{H}^{(0)}) \in \mathcal{F}_\epsilon$ the sequence $\{(\boldsymbol{W}^{(l)}, \boldsymbol{H}^{(l)})\}_{l=0}^{\infty}$ generated by (12) and (13) is contained in a closed and bounded set.

Proof: It suffices for us to show that u_{ik} and v_{kj} in the multiplicative update rule described by (12) and (13) satisfies the conditions of Lemma 2. In the following, we consider only u_{ik} because v_{kj} can be discussed in the same way. First, because $d_1 - 1 \geq 0$ and $d_2 - 1 \leq 0$, we have

$$\frac{\left(\sum_{pq} b_{2pq}(\boldsymbol{W}\boldsymbol{H})^{c_2}_{pq}\right)^{d_2-1}}{\left(\sum_{pq} b_{1pq}(\boldsymbol{W}\boldsymbol{H})^{c_1}_{pq}\right)^{d_1-1}}$$

$$
\begin{aligned}
&\leq \frac{\left(\sum_q b_{2iq}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_2}\right)^{d_2-1}}{\left(\sum_q b_{1iq}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_1}\right)^{d_1-1}} \\
&\leq \frac{\sum_q b_{2iq}^{d_2-1}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_2(d_2-1)}}{\sum_q b_{1iq}^{d_1-1}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_1(d_1-1)}} \\
&= \sum_q \frac{b_{2iq}^{d_2-1}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_2(d_2-1)}}{\sum_s b_{1is}^{d_1-1}(\boldsymbol{W}\boldsymbol{H})_{is}^{c_1(d_1-1)}} \\
&\leq \sum_q \frac{b_{2iq}^{d_2-1}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_2(d_2-1)}}{b_{1iq}^{d_1-1}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_1(d_1-1)}}. \qquad (22)
\end{aligned}
$$

We also have

$$
\frac{\sum_q b_{2iq}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_2-1}H_{kq}}{\sum_q b_{1iq}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_1-1}H_{kq}} \leq \sum_q \frac{b_{2iq}}{b_{1iq}}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_2-c_1}. \qquad (23)
$$

From (22) and (23) we have

$$
\begin{aligned}
&u_{ik}(\boldsymbol{W},\boldsymbol{H}) \\
&\leq W_{ik}\left[-\frac{a_2c_2d_2}{a_1c_1d_1}\sum_q \frac{b_{2iq}^{d_2-1}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_2(d_2-1)}}{b_{1iq}^{d_1-1}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_1(d_1-1)}} \times \sum_q \frac{b_{2iq}}{b_{1iq}}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_2-c_1}\right]^{\frac{1}{\phi_1-\phi_2}} \\
&= W_{ik}\left[-\frac{a_2c_2d_2}{a_1c_1d_1}\sum_q\left(\frac{b_{2iq}^{d_2-1}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_2(d_2-1)}}{b_{1iq}^{d_1-1}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_1(d_1-1)}} \times \sum_s \frac{b_{2is}}{b_{1is}}(\boldsymbol{W}\boldsymbol{H})_{is}^{c_2-c_1}\right)\right]^{\frac{1}{\phi_1-\phi_2}} \\
&\leq W_{ik}\left[-\frac{a_2c_2d_2}{a_1c_1d_1}\sum_q\left(\frac{b_{2iq}^{d_2-1}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_2(d_2-1)}}{b_{1iq}^{d_1-1}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_1(d_1-1)}} \times \frac{b_{2iq}}{b_{1iq}}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_2-c_1}\right)\right]^{\frac{1}{\phi_1-\phi_2}} \\
&\leq W_{ik}\left[-\frac{a_2c_2d_2}{a_1c_1d_1}\sum_q \frac{b_{2iq}^{d_2}}{b_{1iq}^{d_1}(\boldsymbol{W}\boldsymbol{H})_{iq}^{c_1d_1-c_2d_2}}\right]^{\frac{1}{\phi_1-\phi_2}} \\
&\leq W_{ik}\left[-\frac{a_2c_2d_2}{a_1c_1d_1}\sum_q \frac{b_{2iq}^{d_2}}{b_{1iq}^{d_1}(\epsilon W_{ik})^{c_1d_1-c_2d_2}}\right]^{\frac{1}{\phi_1-\phi_2}} \\
&= W_{ik}^{1-\frac{c_1d_1-c_2d_2}{\phi_1-\phi_2}}\left[-\frac{a_2c_2d_2}{a_1c_1d_1}\sum_q \frac{b_{2iq}^{d_2}}{b_{1iq}^{d_1}\epsilon^{c_1d_1-c_2d_2}}\right]^{\frac{1}{\phi_1-\phi_2}}.
\end{aligned}
$$

Because $c_1d_1 - c_2d_2$ is positive due to assumption (10) and $\phi_1 - \phi_2$ is also positive due to Lemma 1, the constant $1 - (c_1d_1 - c_2d_2)/(\phi_1 - \phi_2)$ is less than 1. In addition, the constant

$$
\left[-\frac{c_2e_2l_2}{c_1e_1l_1}\sum_q \frac{b_{2iq}^{d_2}}{b_{1iq}^{d_1}\epsilon^{c_1d_1-c_2d_2}}\right]^{\frac{1}{\phi_1-\phi_2}}
$$

depends neither on $\boldsymbol{W}$ nor on $\boldsymbol{H}$. Therefore, f_{ik} satisfies the conditions of Lemma 2. ∎

VI. Conclusion

For a class of constrained optimization problems which include many NMF optimization problems as special cases, we have given a sufficient condition under which a multiplicative update rule can be obtained. We have also given a sufficient condition under which a modified version of the multiplicative update rule has the global convergence property. A future problem is to extend the results of this paper to the case where the objective function has more than two terms.

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