

A High-Order Proximity-Incorporated Nonnegative Matrix Factorization-based Community Detector: Supplementary File

Zhigang Liu, Xin Luo, *Senior Member, IEEE*

I. INTRODUCTION

THIS is the supplementary file for the paper entitled “A *High-Order Proximity-Incorporated Nonnegative Matrix Factorization-based Community Detector*”. We have put the proof of *Theorem 1* and *Convergence Proof* in Section II.

II. PROOF OF THEOREMS 1 AND CONVERGENCE PROOF

A. Proof of Theorem 1

Proof. We prove the correctness of the learning rules in (23) in the manuscript separately in the following.

a) Updating X : If the learning rule in (23a) in the manuscript converges, then we achieve $X^{(\infty)}=X^{(t+1)}=X^{(t)}=X^{(*)}$, where t denotes the t -th iteration. Thus, for each x_{ik} in X , we have the following inference:

$$\begin{aligned} x_{ik}^{(*)} &= \lim_{t \rightarrow \infty} x_{ik}^{(t)} = x_{ik}^{(t+1)} \\ &= x_{ik}^{(t)} \left(1 - \beta + \beta \frac{\left((1 + \lambda) \tilde{A}X^{(t)} + \mathcal{G}Y + \mathcal{G}U \right)_{sk}}{\left(X^{(t)} \left(X^{(t)} \right)^T X^{(t)} + 2\mathcal{G}X^{(t)} + \lambda \tilde{D}X^{(t)} \right)_{ik}} \right) \\ &\Rightarrow x_{ik}^{(*)} = 0, \text{ or } \left(X^{(*)} \left(X^{(*)} \right)^T X^{(*)} + 2\mathcal{G}X^{(*)} + \lambda \tilde{D}X^{(*)} - (1 + \lambda) \tilde{A}X^{(*)} - \mathcal{G}Y - \mathcal{G}U \right)_{ik} = 0, \end{aligned} \quad (\text{S1})$$

which results in

$$\left(X^{(*)} \left(X^{(*)} \right)^T X^{(*)} + 2\mathcal{G}X^{(*)} + \lambda \tilde{D}X^{(*)} - (1 + \lambda) \tilde{A}X^{(*)} - \mathcal{G}Y - \mathcal{G}U \right)_{ik} x_{ik}^{(*)} = 0, \quad (\text{S2})$$

which is identical with (22a) in the manuscript.

b) Updating Y : If the learning rule in (23b) in the manuscript converges, then we achieve $Y^{(\infty)}=Y^{(t+1)}=Y^{(t)}=Y^{(*)}$, where t denotes the t -th iteration. Thus, for each y_{jk} in Y , we have the following inference:

$$\begin{aligned} y_{jk}^{(*)} &= \lim_{t \rightarrow \infty} y_{jk}^{(t)} = y_{jk}^{(t+1)} = y_{jk}^{(t)} \frac{\left(\tilde{A}U + X \right)_{jk}}{\left(Y^{(t)}U^T U + Y^{(t)} \right)_{jk}} \\ &\Rightarrow y_{jk}^{(*)} = 0, \text{ or } \left(Y^{(*)}U^T U + Y^{(*)} - \tilde{A}U - X \right)_{jk} = 0, \end{aligned} \quad (\text{S3})$$

which results in

$$\left(Y^{(*)}U^T U + Y^{(*)} - \tilde{A}U - X \right)_{jk} y_{jk}^{(*)} = 0, \quad (\text{S4})$$

which is identical with (22b) in the manuscript.

c) Updating U : If the learning rule in (23c) in the manuscript converges, then we achieve $U^{(\infty)}=U^{(t+1)}=U^{(t)}=U^{(*)}$, where t denotes the t -th iteration. Thus, for each u_{sk} in U , we have the following inference:

$$\begin{aligned} u_{sk}^{(*)} &= \lim_{t \rightarrow \infty} u_{sk}^{(t)} = u_{sk}^{(t+1)} = u_{sk}^{(t)} \frac{\left(\tilde{A}^T Y + X \right)_{sk}}{\left(U^{(t)}Y^T Y + U^{(t)} \right)_{sk}} \\ &\Rightarrow u_{sk}^{(*)} = 0, \text{ or } \left(U^{(*)}Y^T Y + U^{(*)} - \tilde{A}^T Y - X \right)_{sk} = 0, \end{aligned} \quad (\text{S5})$$

which results in

$$\left(U^{(*)} Y^T Y + U^{(*)} - \tilde{A}^T Y - X \right)_{sk} u_{sk}^{(*)} = 0, \quad (S6)$$

which is identical with (22c) in the manuscript.

Based on the above analysis, we conclude that converging solutions of X , Y and U satisfy the KKT optimality conditions. ■

B. Convergence Proof

Following [36, 47, 48], we conduct the proof by introducing auxiliary functions for the objective function of optimization problem (19) in the manuscript to help us prove that J_{CGF} is non-increasing during the updating of each single variable. We start the proof by recalling the definition of an auxiliary function [36, 47].

Definition S1. Given a function $\Gamma(x, x^{(t)})$, if it simultaneously fulfills that $\Gamma(x, x^{(t)}) \geq F(x)$ and $\Gamma(x, x) \geq F(x)$, then $\Gamma(x, x^{(t)})$ can be an auxiliary function for $F(x)$.

Based on *Definition S1*, we recall the property of an auxiliary function [36, 47].

Lemma S1. If $\Gamma(x, x^{(t)})$ is an auxiliary function of $F(x)$, then $F(x)$ is non-increasing in each iteration by the following learning rule:

$$x^{(t+1)} = \arg \min_x \Gamma(x, x^{(t)}). \quad (S7)$$

Note that the proof for *Lemma S1* is provided in [47]. Thus, we aim to prove that (23) in the manuscript for X , Y and U is essentially equivalent to (S7) with properly-designed auxiliary functions.

Due to the non-convexity of J_{CGF} , we aim to prove its non-increment with separately X , Y or U under (23) in the manuscript by keeping the other two alternatively fixed, which is consistent with the proof sketch in [36, 47].

a) Updating X : Considering an arbitrary entry x_{ik} in X , we adopt $F(x_{ik})$ to denote the corresponding component from J_{CGF} that is relevant to x_{ik} only. We calculate the first-order and second-order derivatives of $F(x_{ik})$ with respect to x_{ik} , i.e.,

$$F'(x_{ik}) = \frac{\partial J_{CGF}}{\partial x_{ik}} = (-9Y - 9U + XX^T X - \tilde{A}X + \lambda \tilde{L}X)_{ik} + 29x_{ik}, \quad (S8)$$

$$F''(x_{ik}) = \frac{\partial^2 J_{CGF}}{\partial x_{ik}^2} = (X^T X)_{kk} + (XX^T - \tilde{A} + \lambda \tilde{L})_{ii} + 29 + x_{ik}^2. \quad (S9)$$

Lemma S2. The following $\Gamma(x_{ik}, x_{ik}^{(t)})$ is an auxiliary function for $F(x_{ik})$.

$$\Gamma(x_{ik}, x_{ik}^{(t)}) = F(x_{ik}^{(t)}) + F'(x_{ik}^{(t)})(x_{ik} - x_{ik}^{(t)}) + \frac{(XX^T X + \lambda \tilde{D}X)_{ik} + 29x_{ik}^{(t)}}{2\beta x_{ik}^{(t)}} (x_{ik} - x_{ik}^{(t)})^2. \quad (S10)$$

Proof. Note that with (S10) $\Gamma(x_{ik}, x_{ik}) = F(x_{ik})$ evidently holds. Thus, we aim to prove that $\Gamma(x_{ik}, x_{ik}^{(t)}) \geq F(x_{ik})$. To achieve this objective, we expand $F(x_{ik})$ to its second-order Taylor series at the state point $x_{ik}^{(t)}$ as:

$$F(x_{ik}) = F(x_{ik}^{(t)}) + F'(x_{ik}^{(t)})(x_{ik} - x_{ik}^{(t)}) + \frac{1}{2} \left((X^T X)_{kk} + (XX^T - \tilde{A} + \lambda \tilde{L})_{ii} + 29 + x_{ik}^2 \right) (x_{ik} - x_{ik}^{(t)})^2. \quad (S11)$$

By combining (S10) and (S11), we see that the desired condition of $\Gamma(x_{ik}, x_{ik}^{(t)}) \geq F(x_{ik})$ is equivalent to the following condition:

$$\frac{(XX^T X + \lambda \tilde{D}X)_{ik} + 29x_{ik}^{(t)}}{\beta x_{ik}^{(t)}} \geq (X^T X)_{kk} + (XX^T + \lambda \tilde{D} - (1 + \lambda) \tilde{A})_{ii} + 29 + (x_{ik}^{(t)})^2 \quad (S12)$$

Since $x_{ik}^{(t)} \geq 0^1$, (S12) can be reduced into the following form:

$$\frac{1}{\beta} (XX^T X + \lambda \tilde{D}X)_{ik} \geq x_{ik}^{(t)} (X^T X)_{kk} + (XX^T + \lambda \tilde{D} - (1 + \lambda) \tilde{A})_{ii} x_{ik}^{(t)} + (x_{ik}^{(t)})^3. \quad (S13)$$

It is easy to show that

$$(XX^T X)_{ik} = \sum_{f=1}^K (x_{if} (X^T X)_{fk}) = \sum_{f=1, f \neq k}^K (x_{if} (X^T X)_{fk}) + x_{ik} (X^T X)_{kk} \geq x_{ik} (X^T X)_{kk}. \quad (S14)$$

Similarly, we have

$$(XX^T X)_{ik} \geq (XX^T)_{ii} x_{ik}, \quad (S15)$$

and

$$(XX^T X)_{ik} \geq x_{ik}^3. \quad (S16)$$

By combining (S15)-(S16), we have

¹ Please note that if $x_{ik}^{(t)}$ goes to zero after the t -th iteration, then it will keep zero constantly with the learning scheme (22) in the follow-up iterations, which will not affect the convergence of the learning algorithm. Therefore, without loss of generality, we only take into account the case of $x_{ik}^{(t)} > 0$ in our proof. Similarly, only the case of $y_{jk}^{(t)} > 0$ or $u_{sk}^{(t)} > 0$ is taken into consideration when we present the proof of **Updating Y** and **Updating U** later, respectively.

$$\left(XX^T X\right)_{ik} \geq \frac{1}{3} \left(x_{ik} \left(X^T X \right)_{kk} + \left(XX^T \right)_{ii} x_{ik} + x_{ik}^3 \right). \quad (S17)$$

On the other hand, we have

$$\lambda \left(\tilde{D}X \right)_{ik} = \lambda \sum_{h=1}^n \tilde{D}_{ih} x_{hk} = \lambda \sum_{h=1, h \neq i}^n \tilde{D}_{ih} x_{hk} + \lambda \tilde{D}_{ii} x_{ik} \geq \lambda \tilde{D}_{ii} x_{ik} \geq \lambda \left(\tilde{D} - (1+\lambda) \tilde{A} \right)_{ii} x_{ik}. \quad (S18)$$

Based on the inferences in (S17) and (S18), we conclude that (S13) holds when $0 < \beta \leq 1/3$, resulting in the establishment of (S12). Note that it is hard to rigorously show that (S13) still holds when $1/3 < \beta \leq 1$. But in fact, (S13) most likely would hold when $1/3 < \beta \leq 1$, since in the shrinkage process of (S14)-(S18) we cast away many positive terms that ensures that (S13) holds. Besides, the empirical convergence analysis later has also confirmed this inference. Therefore, we have $\Gamma(x_{ik}, x_{ik}^{(t)}) \geq F(x_{ik})$, which makes $\Gamma(x_{ik}, x_{ik}^{(t)})$ be an auxiliary function of $F(x_{ik})$. \square

Based on *Lemmas S1* and *S2*, we then have the following theorem.

Theorem S1. The value of J_{CGF} in (19) in the manuscript keeps non-increasing when updating X by the learning rule (23a).

Proof. It is equivalent to proving that the learning rule in (S7) is consistent with that in (23a). Thus, by replacing $\Gamma(x_{ik}, x_{ik}^{(t)})$ in (S7) with the auxiliary function in (S10), we have:

$$\begin{aligned} x_{ik}^{(t+1)} &= \arg \min_{x_{ik}} \Gamma(x_{ik}, x_{ik}^{(t)}) \\ \Rightarrow F'(x_{ik}^{(t)}) + \frac{(XX^T X + \lambda \tilde{D}X)_{ik} + 2\mathcal{G}x_{ik}^{(t)}}{\beta x_{ik}^{(t)}} (x_{ik} - x_{ik}^{(t)}) &= 0 \\ \Rightarrow x_{ik} &= x_{ik}^{(t)} - x_{ik}^{(t)} \frac{\beta F'(x_{ik}^{(t)})}{(XX^T X + \lambda \tilde{D}X)_{ik} + 2\mathcal{G}x_{ik}^{(t)}} \\ \Rightarrow x_{ik}^{(t+1)} &= x_{ik}^{(t)} \left(1 - \beta + \beta \frac{((1+\lambda)\tilde{A}X + \mathcal{G}Y + \mathcal{G}U)_{ik}}{(XX^T X + \lambda \tilde{D}X + 2\mathcal{G}X)_{ik}} \right), \end{aligned} \quad (S19)$$

which is identical with the learning rule in (23a). Note that x_{ik} is an arbitrary entry of X . Hence, $\forall i \in \{1, 2, \dots, n\}, k \in \{1, 2, \dots, K\}$, $F(x_{ik})$ is non-increasing with the learning scheme (23a) as Y and U are alternatively fixed. Based on the inferences above, we conclude that J_{CGF} is non-increasing when updating X by the learning rule (23a). Hence, *Theorem S1* stands. \blacksquare

b) Updating Y : By analogy, considering an arbitrary entry y_{jk} in Y , we adopt the function $F(y_{jk})$ to denote the corresponding component from J_{CGF} that is relevant to y_{jk} only. Then, we have the first-order and second-order derivatives of $F(y_{jk})$ with respect to y_{jk} , i.e.,

$$F'(y_{jk}) = \frac{\partial J_{CGF}}{\partial y_{jk}} = (\mathcal{G}YU^T U - \mathcal{G}\tilde{A}U - \mathcal{G}X)_{jk} + \mathcal{G}y_{jk}, \quad (S20)$$

$$F''(y_{jk}) = \frac{\partial^2 J_{CGF}}{\partial y_{jk}^2} = \mathcal{G}(U^T U)_{kk} + \mathcal{G}. \quad (S21)$$

Lemma S3. The following $\Gamma(y_{jk}, y_{jk}^{(t)})$ is an auxiliary function for $F(y_{jk})$.

$$\Gamma(y_{jk}, y_{jk}^{(t)}) = F(y_{jk}^{(t)}) + F'(y_{jk}^{(t)}) (y_{jk} - y_{jk}^{(t)}) + \frac{\mathcal{G}(YU^T U)_{jk} + \mathcal{G}y_{jk}^{(t)}}{2y_{jk}^{(t)}} (y_{jk} - y_{jk}^{(t)})^2. \quad (S22)$$

Proof. With (S18), $\Gamma(y_{jk}, y_{jk}) = F(y_{jk})$ holds. Next, we aim to prove that $\Gamma(y_{jk}, y_{jk}^{(t)}) \geq F(y_{jk})$. To do this, we expand $F(y_{jk})$ to its second-order Taylor series at the state point $y_{jk}^{(t)}$ as:

$$F(y_{jk}) = F(y_{jk}^{(t)}) + F'(y_{jk}^{(t)}) (y_{jk} - y_{jk}^{(t)}) + \frac{1}{2} (\mathcal{G}(U^T U)_{kk} + \mathcal{G}) (y_{jk} - y_{jk}^{(t)})^2. \quad (S23)$$

Combining (S22) and (S23), we see that the desired condition of $\Gamma(y_{jk}, y_{jk}^{(t)}) \geq F(y_{jk})$ is equivalent to the following condition:

$$(\mathcal{G}(YU^T U)_{jk} + \mathcal{G}y_{jk}^{(t)}) / y_{jk}^{(t)} \geq \mathcal{G}(U^T U)_{kk} + \mathcal{G}. \quad (S24)$$

Since $y_{jk}^{(t)} \geq 0$ and $\mathcal{G} > 0$, (S24) can be reduced into the following form:

$$(YU^T U)_{jk} \geq y_{jk}^{(t)} (U^T U)_{kk}. \quad (S25)$$

To prove (S25), we have the following inferences:

$$(YU^T U)_{jk} = \sum_{f=1}^K y_{jf}^{(t)} (U^T U)_{fk} = \sum_{f=1, f \neq k}^K y_{jf}^{(t)} (U^T U)_{fk} + y_{jk}^{(t)} (U^T U)_{kk} \geq y_{jk}^{(t)} (U^T U)_{kk}. \quad (S26)$$

Hence, (S24) holds based on (S26), thus making $\Gamma(y_{jk}, y_{jk}^{(t)})$ be an auxiliary function of $F(y_{jk})$. \square

Based on *Lemmas* S1 and S3, we then have the following theorem.

Theorem S2. The value of J_{CGF} in (19) in the manuscript keeps non-increasing when updating Y by the learning rule (23b).

Proof. It is equivalent to proving that the learning rule in (S7) is consistent with that in (23b). By replacing $\Gamma(y_{jk}, y_{jk}^{(i)})$ in (S7) with the auxiliary function in (S23), we have:

$$\begin{aligned} y_{jk}^{(t+1)} &= \arg \min_{y_{jk}} \Gamma(y_{jk}, y_{jk}^{(t)}) \\ \Rightarrow F'(y_{jk}^{(t)}) + \frac{\mathcal{G}(YU^T U)_{jk} + \mathcal{G}y_{jk}^{(t)}}{y_{jk}^{(t)}} (y_{jk} - y_{jk}^{(t)}) &= 0 \\ \Rightarrow y_{jk} &= y_{jk}^{(t)} - y_{jk}^{(t)} \frac{F'(y_{jk}^{(t)})}{\mathcal{G}(YU^T U)_{jk} + \mathcal{G}y_{jk}^{(t)}} \Rightarrow y_{jk}^{(t+1)} = y_{jk}^{(t)} \frac{(\tilde{A}U + X)_{jk}}{(YU^T U + Y)_{jk}}, \end{aligned} \quad (S27)$$

which is identical with the learning rule in (23b). Similarly, $\forall j \in \{1, 2, \dots, n\}, k \in \{1, 2, \dots, K\}$, $F(y_{jk})$ keeps non-increasing under the learning scheme (23b) as X and U are alternatively fixed. Thus, we conclude that J_{CGF} keeps non-increasing when updating Y by the learning rule (23b), and *Theorem* S2 stands. ■

c) Updating U : Similarly, considering an arbitrary entry u_{sk} in U , we adopt $F(u_{sk})$ to denote the corresponding component from J_{CGF} that is relevant to u_{sk} only. Then, we have the first-order and second-order derivatives of $F(u_{sk})$ with respect to u_{sk} , i.e.,

$$F'(u_{sk}) = \frac{\partial J_{CGF}}{\partial u_{sk}} = (\mathcal{G}UY^T Y - \mathcal{G}\tilde{A}^T Y - \mathcal{G}X)_{sk} + \mathcal{G}u_{sk}, \quad (S28)$$

$$F''(u_{sk}) = \frac{\partial^2 J_{CGF}}{\partial u_{sk}^2} = \mathcal{G}(Y^T Y)_{kk} + \mathcal{G}. \quad (S29)$$

Next, we build an auxiliary function for $F(u_{sk})$.

Lemma S4. The following $\Gamma(u_{sk}, u_{sk}^{(i)})$ is an auxiliary function for $F(u_{sk})$.

$$\Gamma(u_{sk}, u_{sk}^{(i)}) = F(u_{sk}^{(i)}) + F'(u_{sk}^{(i)})(u_{sk} - u_{sk}^{(i)}) + \frac{\mathcal{G}(UY^T Y)_{sk} + \mathcal{G}u_{sk}^{(i)}}{2u_{sk}^{(i)}} (u_{sk} - u_{sk}^{(i)})^2. \quad (S30)$$

Proof. Based on (S30), $\Gamma(u_{sk}, u_{sk}) = F(u_{sk})$ holds. Next, we need to prove that $\Gamma(u_{sk}, u_{sk}^{(i)}) \geq F(u_{sk})$. To do this, we expand $F(u_{sk})$ to its second-order Taylor series at the state point $u_{sk}^{(i)}$, i.e.,

$$F(u_{sk}) = F(u_{sk}^{(i)}) + F'(u_{sk}^{(i)})(u_{sk} - u_{sk}^{(i)}) + \frac{1}{2}(\mathcal{G}(Y^T Y)_{kk} + \mathcal{G})(u_{sk} - u_{sk}^{(i)})^2. \quad (S31)$$

By combining (S30) and (S31), we see that the desired condition of $\Gamma(u_{sk}, u_{sk}^{(i)}) \geq F(u_{sk})$ is equivalent to the following condition:

$$(\mathcal{G}(UY^T Y)_{sk} + \mathcal{G}u_{sk}^{(i)})/u_{sk}^{(i)} \geq \mathcal{G}(Y^T Y)_{kk} + \mathcal{G}. \quad (S32)$$

Since $u_{sk}^{(i)} \geq 0$ and $\mathcal{G} > 0$, (S32) can be reduced into the following form:

$$(UY^T Y)_{sk} \geq u_{sk}^{(i)} (Y^T Y)_{kk}. \quad (S33)$$

To prove (S33), we have the following inferences:

$$(UY^T Y)_{sk} = \sum_{f=1}^K u_{sf}^{(i)} (Y^T Y)_{fk} = \sum_{f=1, f \neq k}^K u_{sf}^{(i)} (Y^T Y)_{fk} + u_{sk}^{(i)} (Y^T Y)_{kk} \geq u_{sk}^{(i)} (Y^T Y)_{kk}. \quad (S34)$$

Hence, (S34) holds and we have $\Gamma(u_{sk}, u_{sk}^{(i)}) \geq F(u_{sk})$, which makes $\Gamma(u_{sk}, u_{sk}^{(i)})$ be an auxiliary function of $F(u_{sk})$. □

Based on *Lemmas* S1 and S4, we can prove the convergence of the learning rule (23c) in the manuscript.

Theorem S3. The value of J_{CGF} in (19) in the manuscript keeps non-increasing when updating U by the learning rule (23c).

Proof. It is equivalent to proving that the learning rule in (S7) is consistent with that in (23c). By replacing $\Gamma(u_{sk}, u_{sk}^{(i)})$ in (S7) with the auxiliary function in (S30), we have:

$$\begin{aligned} u_{sk}^{(t+1)} &= \arg \min_{u_{sk}} \Gamma(u_{sk}, u_{sk}^{(t)}), \\ \Rightarrow F'(u_{sk}^{(t)}) + \frac{\mathcal{G}(UY^T Y)_{sk} + \mathcal{G}u_{sk}^{(t)}}{u_{sk}^{(t)}} (u_{sk} - u_{sk}^{(t)}) &= 0, \\ \Rightarrow u_{sk} &= u_{sk}^{(t)} - u_{sk}^{(t)} \frac{F'(u_{sk}^{(t)})}{\mathcal{G}(UY^T Y)_{sk} + \mathcal{G}u_{sk}^{(t)}} \Rightarrow u_{sk}^{(t+1)} = u_{sk}^{(t)} \frac{(\tilde{A}^T Y + X)_{sk}}{(UY^T Y + U)_{sk}}, \end{aligned} \quad (S35)$$

which is identical with the learning rule in (23c). Similarly, $\forall s \in \{1, 2, \dots, n\}, k \in \{1, 2, \dots, K\}$, $F(u_{sk})$ is non-increasing with the learning scheme (23c) as X and Y are alternatively fixed. Thus, we conclude that J_{CGF} keeps non-increasing when updating U by the learning rule (23c), and *Theorem* S3 stands. ■

With *Theorems* S1-S3, we conclude that the convergence of the HOP-NMF-based community detector with the learning scheme (23) in the manuscript is guaranteed. Besides, with *Theorem* 1 in the manuscript, we have that the solution sequences of the CGF algorithm fulfils the KKT conditions, thereby making it converge to KKT stationary points of its learning objective.