A Proofs of Convergence

We need solve following function in order to update G, with other parameters fixed.

$$\begin{aligned}\min_{G\geqslant 0}\ L(G) &= \parallel G - EC^{\mathrm{T}} \parallel_F^2 - \lambda\, tr(G^{\mathrm{T}}\, B\, G) \\ &= \parallel G - EC^{\mathrm{T}} \parallel_F^2 - \lambda\, tr(G^{\mathrm{T}}\, (A-P)\, G) \\ &s.t.,\ tr(G^{\mathrm{T}}\, G) = N\end{aligned} \tag{A1}$$

where the element of P is $\frac{k_i k_j}{2m}$, and it is a NP-hard problem because of the constraint of G. To this end, the regularization coefficient α is introduced for relaxing the constraint to $G^{\mathrm{T}}\, G = I$, the function (A1) can be rewritten as:

$$\begin{aligned}\min_{G\geqslant 0}\ L(G) = &\parallel G - EC^{\mathrm{T}} \parallel_F^2 + \alpha \parallel G^{\mathrm{T}}\, G - I \parallel_F^2 \\ &- \lambda\, tr(G^{\mathrm{T}}\, AG) + \lambda\, tr(G^{\mathrm{T}}\, PG)\end{aligned} \tag{A2}$$

Let ψ_{ij} be the lagrange multiplier for constraint $e_{ij} \geqslant 0$, and $\Psi = [\psi_{ij}]$, the Lagrange $\mathcal{L}$ is

$$\begin{aligned}\mathcal{L} = &tr(GG^{\mathrm{T}} - 2GCE^{\mathrm{T}} + EC^{\mathrm{T}}CE^{\mathrm{T}}) \\ &+ \alpha\, tr(G^{\mathrm{T}}GG^{\mathrm{T}}G - 2G^{\mathrm{T}}G + I) + tr(\Psi G^{\mathrm{T}}) \\ &- \lambda\, tr(G^{\mathrm{T}}\, AG) + \lambda\, tr(G^{\mathrm{T}}\, PG)\end{aligned} \tag{A3}$$

where the formula applies the matrix properties $\|X\|_F^2 = tr(X^{\mathrm{T}}X)$, and let the the partial derivative of Lagrange $\mathcal{L}$ with respect to G to 0, we have:

$$\Psi = -2G + 2EC^{\mathrm{T}} - 4\alpha GG^{\mathrm{T}}G + 4\alpha G + 2\lambda AG - 2\lambda PG \tag{A4}$$

Using the KKT condition $\psi_{ij} g_{ij} = 0$, we get the following equation for g_{ij}:

$$(-2G + 2EC^{\mathrm{T}} - 4\alpha GG^{\mathrm{T}}G + 4\alpha G + 2\lambda AG - 2\lambda PG)_{ij} g_{ij} = 0. \tag{A5}$$

The equation leads to the following updating rule:

$$g_{ij} \longleftarrow g_{ij} \sqrt{\frac{-2\lambda PG + \sqrt{\varDelta}}{8\,\alpha\, GG^{\mathrm{T}}G}}_{ij} \tag{A6}$$

where $\varDelta = 2\lambda(PG)_{ij}\, 2\lambda(PG)_{ij} + 16\alpha(GG^{\mathrm{T}}G)_{ij}\, (2\lambda(PG) + 2EC^{\mathrm{T}} + (4\alpha - 2)G)_{ij}$

Regarding these updating rules, we have the following theorem:

Theorem 1. *The object function (9) is nonincreasing under the updating rules in (10) and (11).*

Since the second term in (9) is only related to G, we have the same update formula for E and C in (9) as in the original NMF. Consequently, we can use the convergence proof of NMF to show that (9) is nonincreasing under the update steps in (10). More details please refer to Ref. [32]. Now, we need to prove the optimization problem (A2) is nonincreasing under the iterative updating rule (11). With regard to this, we will utilize an auxiliary function same as that used in Ref. [32]. We begin with the definition of the auxiliary function.

Definition 1. $D(G, G^{'})$ *is an auxiliary function for function* $L(G)$*, if the conditions* $D(G, G^{'} \geqslant L(G),\ D(G, G) = L(G)$ *are satisfied.*

The auxiliary function gives rise to the following lemma:

Lemma 1. *If D is the auxiliary function of L, then L is nonincreasing under the update* $G^{(t+1)} = arg\min_{G} D(G, G^{t})$.

Proof. $L(G^{(t+1)}) \leqslant D(G^{(t+1)}, G^{(t)}) \leqslant D(G^{(t)}, G^{(t)}) \leqslant L(G^{(t)})$

Now, we will show that the update step for G in (11) is exactly the update in lemma 1 with a proper auxiliary function.

Lemma 2. *Function*

$$\begin{aligned} D(G,G^{'}) = & -(2\alpha-1)(tr(G^{'\mathrm{T}}Z)+tr(Z^{\mathrm{T}}G^{'})+tr(G^{'\mathrm{T}}G^{'})) \\ & -2(tr(CE^{'\mathrm{T}}Z)+tr(CE^{'\mathrm{T}}G^{'}))+\alpha tr(VG^{'\mathrm{T}}G^{'}G^{'\mathrm{T}}) \\ & -\lambda(tr(G^{'\mathrm{T}}AZ)+tr(Z^{\mathrm{T}}AG^{'})+tr(G^{'\mathrm{T}}AG^{'})) \\ & +\frac{1}{2}\lambda(tr(Y^{\mathrm{T}}PG^{'})+tr(G^{'\mathrm{T}}PY)) \end{aligned} \tag{A7}$$

is the auxiliary function for $L(G)$ in (A2), where $Z_{ij} = G^{'}_{ij}\ln\dfrac{G_{ij}}{G^{'}_{ij}}$, $V_{ij} = \dfrac{G^{4}_{ij}}{G^{'3}_{ij}}$ *and* $Y_{ij} = \dfrac{G^{2}_{ij}}{G^{'}_{ij}}$.

Proof. To search the proper auxiliary function for $L(G)$ in equation (A2) is equivalent to find the auxiliary function for $\mathcal{L}$ in equation (A3) without the term $tr(\Psi G^{\mathrm{T}})$.

According to lemma 4 in Ref. [31], we have

$$-(2\alpha-1)tr(G^{\mathrm{T}}G) \leqslant -(2\alpha-1)(tr(G^{'\mathrm{T}}Z)+tr(Z^{\mathrm{T}}G^{'})+tr(G^{'\mathrm{T}}G^{'})), \tag{A8}$$

and

$$-\lambda tr(G^{\mathrm{T}}AG) \leqslant -\lambda(tr(G^{'\mathrm{T}}AZ)+tr(Z^{\mathrm{T}}AG^{'})+tr(G^{'\mathrm{T}}AG^{'})). \tag{A9}$$

According to lemma 2 in Ref. [31], we have

$$-2tr(GCE^{'\mathrm{T}}) \leqslant -2(tr(CE^{'\mathrm{T}}Z)+tr(CE^{'\mathrm{T}}G^{'})). \tag{A10}$$

According to lemma 6 and 7 in Ref. [31], we have

$$\alpha tr(G^{\mathrm{T}}GG^{\mathrm{T}}G) \leqslant \alpha tr(UG^{'\mathrm{T}}G^{'}) \leqslant \alpha tr(VG^{'\mathrm{T}}G^{'}G^{'\mathrm{T}}), \tag{A11}$$

where $U_{ij} = \dfrac{(G^{\mathrm{T}}G)^{2}_{ij}}{(G^{'\mathrm{T}}G^{'})_{ij}}$ and $V_{ij} = \dfrac{G^{4}_{ij}}{G^{'3}_{ij}}$.

According to lemma 6 in Ref. [31], we have

$$\lambda tr(G^{\mathrm{T}}PG) \leqslant \frac{1}{2}\lambda(tr(Y^{\mathrm{T}}PG^{'})+tr(G^{'\mathrm{T}}PY)). \tag{A12}$$

Thus, the auxiliary function (A7) holds, the update step in (A6) is convergent for G.

Based on the lemma 1 and lemma 2, we can now demonstrate the convergence of theorem 1.

Proof. Since we have the auxiliary function $D(G, G^{'})$ in (A7) of $L(G)$, and in order to solve the $arg \min_{G} D(G, G^{t})$, we can set the partial derivative of $D(G, G^{'})$ with respect to G to 0.

$$
\begin{aligned}
\frac{\partial D(G, G^{'})}{\partial G_{ij}} =& 4\alpha(G^{'} G^{'\mathrm{T}} G^{'})_{ij} G_{ij}^{4} + 2\lambda(PG^{'})_{ij} G_{ij}^{'2} G_{ij}^{2} \\
& - 2\lambda(AG^{'})_{ij} G_{ij}^{'4} - 2(EC^{\mathrm{T}})_{ij} G_{ij}^{'4} \\
& - (4\alpha - 2) G_{ij}^{'4} = 0.
\end{aligned} \tag{A13}
$$

Finally, the solution of equation (A13) is obtained, which is same as (11). Based on lemma 1, we have proved that the object function (9) is nonincreasing under the updating rules in (10) and (11).