

## Subsection 4.2 (with Details)

Fixing kernel matrices, the updating rules are given below:

$$\mathbf{V}^{(t+1)} = \arg \min_{\|\mathbf{V}_i\|_2^2 < \tau, \forall i} \mathcal{L}(\tilde{\mathbf{H}}^{(t)}, \mathbf{V}; \boldsymbol{\Lambda}^{(t)}) + \frac{\xi^{(t)}}{2} \|\mathbf{V} - \mathbf{V}^{(t)}\|_F^2 \quad (8)$$

$$\tilde{\mathbf{H}}^{(t+1)} = \arg \min \mathcal{L}(\tilde{\mathbf{H}}, \mathbf{V}^{(t+1)}; \boldsymbol{\Lambda}^{(t)}) \quad (9)$$

$$\boldsymbol{\Lambda}^{(t+1)} = \boldsymbol{\Lambda}^{(t)} + \rho(\mathbf{V}^{(t+1)} - \tilde{\mathbf{H}}^{(t+1)}) \quad (10)$$

$$\xi^{(t+1)} = \frac{6}{\rho} \cdot \mathcal{J}(\tilde{\mathbf{H}}^{(t+1)}, \mathbf{B}, \mathbf{C}, \mathbf{V}^{(t+1)}) \quad (11)$$

$$\mathcal{L}(\tilde{\mathbf{H}}, \tilde{\mathbf{B}}, \tilde{\mathbf{C}}, \mathbf{V}; \boldsymbol{\Lambda}) = \mathcal{J}(\tilde{\mathbf{H}}, \tilde{\mathbf{B}}, \tilde{\mathbf{C}}, \mathbf{V}) + \frac{\rho}{2} \|\mathbf{V} - \tilde{\mathbf{H}} + \boldsymbol{\Lambda}/\rho\|_F^2 \quad (12)$$

$\mathcal{L}(\tilde{\mathbf{H}}, \tilde{\mathbf{B}}, \tilde{\mathbf{C}}, \mathbf{V}; \boldsymbol{\Lambda})$  is the augmented Lagrangian. Note that, proximal term  $\|\mathbf{V} - \mathbf{V}^{(t)}\|_F^2$  and penalty parameter  $\beta^{(t)}$  are added according to the study [Lu *et al.*, 2017]. The optimization w.r.t.  $\mathbf{V}$  can be decomposed into  $k$  separable problems, each of which can be solved using gradient projection:

$$\begin{aligned} \mathbf{V}_{[i]}^{(r+1)} &= \text{proj}_{\mathbf{V}}(\mathbf{V}_{[i]}^{(r)} - \tau \nabla_{\mathbf{V}}[\mathcal{L} + \frac{\xi^{(t)}}{2} \|\mathbf{V} - \mathbf{V}^{(t)}\|_F^2]_{[i]}^{(r)}) \\ &= \text{proj}_{\mathbf{V}}(\mathbf{V}_{[i]}^{(r)} - \tau(\mathbf{A}_V^{(t)} \mathbf{V}_{[i]}^{(r)} - \mathbf{B}_V^{(t)})), \end{aligned} \quad (13)$$

$$\mathbf{A}_V^{(t)} = \tilde{\mathbf{B}}^T \tilde{\mathbf{H}}^T \tilde{\mathbf{H}} \tilde{\mathbf{B}} + \tilde{\mathbf{C}}^T \tilde{\mathbf{H}}^T \tilde{\mathbf{H}} \tilde{\mathbf{C}} + (\frac{\xi^{(t)}}{2} + 1) \mathbf{I} \quad (14)$$

$$\mathbf{B}_V^{(t)} = \tilde{\mathbf{M}}^T \tilde{\mathbf{H}} \tilde{\mathbf{B}} + \tilde{\mathbf{S}}^T \tilde{\mathbf{H}} \tilde{\mathbf{C}} + \tilde{\mathbf{H}} + \frac{\xi^{(t)}}{2} \mathbf{H}^{(t)} - \boldsymbol{\Lambda}/\rho \quad (15)$$

$$\text{proj}_{\mathbf{V}}(\mathbf{w}) = \sqrt{\tau} \mathbf{w} / \max\{\sqrt{\tau}, \|\mathbf{w}\|_2\}, \forall \mathbf{w} \in \mathbb{R}^n \quad (16)$$

where  $r$  is the inner-iteration number,  $\alpha$  is the step size and  $\mathbf{V}_{[i]}$  denotes the  $i^{th}$  column of matrix  $\mathbf{V}$ . For a given vector  $\mathbf{w}$ ,  $\text{proj}_{\mathbf{V}}(\cdot)$  projects it onto the feasible set of  $\mathbf{V}_{[i]}$ .  $\tilde{\mathbf{H}}$  can be solved via 1<sup>st</sup>-order method, whose gradient is:

$$\begin{aligned} \nabla_{\tilde{\mathbf{H}}} \mathcal{L} &= \nabla_{\tilde{\mathbf{H}}} \mathcal{J} + \frac{\rho}{2} \nabla_{\tilde{\mathbf{H}}} \|\mathbf{V} - \tilde{\mathbf{H}} + \boldsymbol{\Lambda}/\rho\|_F^2 \\ &= \tilde{\mathbf{H}} \tilde{\mathbf{B}} \mathbf{V}^{(t+1)T} \mathbf{V}^{(t+1)} \tilde{\mathbf{B}}^T - \tilde{\mathbf{M}} \mathbf{V}^{(t+1)} \tilde{\mathbf{B}}^T + \tilde{\mathbf{E}} \tilde{\mathbf{D}}_p \tilde{\mathbf{E}} \tilde{\mathbf{H}} \tilde{\mathbf{D}}_p \\ &\quad + \tilde{\mathbf{H}} \tilde{\mathbf{C}} \mathbf{V}^{(t+1)T} \mathbf{V}^{(t+1)} \tilde{\mathbf{C}}^T - \tilde{\mathbf{S}} \mathbf{V}^{(t+1)} \tilde{\mathbf{C}}^T + \tilde{\mathbf{E}} \tilde{\mathbf{D}}_q \tilde{\mathbf{E}} \tilde{\mathbf{H}} \tilde{\mathbf{D}}_q \\ &\quad + \rho(\tilde{\mathbf{H}} - \mathbf{V}^{(t+1)} - \boldsymbol{\Lambda}^{(t)}/\rho) + 2\tilde{\mathbf{E}}^T \tilde{\mathbf{E}} \tilde{\mathbf{H}} \\ &= (\tilde{\mathbf{H}} \tilde{\mathbf{B}} \mathbf{V}^{(t+1)T} - \tilde{\mathbf{M}} \mathbf{V}^{(t+1)} \tilde{\mathbf{B}}^T + \tilde{\mathbf{E}} \mathcal{R}_p(\tilde{\mathbf{E}} \tilde{\mathbf{H}})) \\ &\quad + (\tilde{\mathbf{H}} \tilde{\mathbf{C}} \mathbf{V}^{(t+1)T} - \tilde{\mathbf{S}} \mathbf{V}^{(t+1)} \tilde{\mathbf{C}}^T + \tilde{\mathbf{E}} \mathcal{R}_q(\tilde{\mathbf{E}} \tilde{\mathbf{H}})) \\ &\quad + \rho(\tilde{\mathbf{H}} - \mathbf{V}^{(t+1)} - \boldsymbol{\Lambda}^{(t)}/\rho) + 2\tilde{\mathbf{E}}^T \tilde{\mathbf{E}} \tilde{\mathbf{H}}, \end{aligned} \quad (17)$$

as  $\mathbf{D}_p = \mathbf{D}_p^{-1}$  and  $\mathbf{D}_q = \mathbf{D}_q^{-1}$ .

## References

[Lu *et al.*, 2017] Songtao Lu, Mingyi Hong, and Zhengdao Wang. A nonconvex splitting method for symmetric non-negative matrix factorization: Convergence analysis and optimality. *IEEE Trans. on Signal Processing*, 2017.