

Supplementary Material for (H)GIR-MRF

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I. DERIVATION OF ALGORITHM 1

Rewrite the minimization model of structured graph learning as follows:

$$\begin{aligned} \min_{\mathbf{W}} Tr(\mathbf{W}^T \mathbf{D}^x) + \left\| \mathbf{W} \boldsymbol{\alpha}^{\frac{1}{2}} \right\|_F^2 + \beta g(\boldsymbol{\varepsilon}) \\ s.t. \mathbf{W} \geq 0, \mathbf{W}^T \mathbf{1}_{N_S} = \mathbf{1}_{N_S}, \mathbf{X} = \mathbf{XW} + \boldsymbol{\varepsilon}. \end{aligned} \quad (1)$$

Problem (1) can be efficiently solved by using the alternating direction method of multipliers (ADMM). First, we introduce an auxiliary variable $\mathbf{S} \in \mathbb{R}^{N_S \times N_S}$, and rewrite the model (1) as the minimization of

$$\begin{aligned} \mathcal{L}(\boldsymbol{\varepsilon}, \mathbf{S}, \mathbf{W}, \mathbf{R}_1, \mathbf{R}_2) = Tr(\mathbf{W}^T \mathbf{D}^x) + \left\| \mathbf{W} \boldsymbol{\alpha}^{\frac{1}{2}} \right\|_F^2 + \beta g(\boldsymbol{\varepsilon}) \\ + Tr(\mathbf{R}_1^T (\mathbf{W} - \mathbf{S})) + Tr(\mathbf{R}_2^T (\mathbf{X} - \mathbf{XS} - \boldsymbol{\varepsilon})) \\ + \frac{\mu_1}{2} \left\| \mathbf{W} - \mathbf{S} \right\|_F^2 + \frac{\mu_2}{2} \left\| \mathbf{X} - \mathbf{XS} - \boldsymbol{\varepsilon} \right\|_F^2 \\ s.t. \mathbf{W} \geq 0, \mathbf{W}^T \mathbf{1}_{N_S} = \mathbf{1}_{N_S}, \end{aligned} \quad (2)$$

where $\mathbf{R}_1 \in \mathbb{R}^{N_S \times N_S}$ and $\mathbf{R}_2 \in \mathbb{R}^{3C_X \times N_S}$ are two Lagrangian multipliers, and $\mu_1, \mu_2 > 0$ are two penalty parameters. Then the alternating direction method (ADM) can be used to solve the minimization of (2) by iteratively updating one variable at a time and fixing the others. ADM separates (2) into $\boldsymbol{\varepsilon}$ -subproblem, \mathbf{S} -subproblem and \mathbf{W} -subproblem.

$\boldsymbol{\varepsilon}$ -subproblem: given the current points $(\boldsymbol{\varepsilon}^{(t)}, \mathbf{S}^{(t)}, \mathbf{W}^{(t)}, \mathbf{R}_1^{(t)}, \mathbf{R}_2^{(t)})$ at the t -th iteration, the minimization of (2) with respect to $\boldsymbol{\varepsilon}$ can be formulated as follows by fixing the unrelated terms

$$\begin{aligned} \boldsymbol{\varepsilon}^{(t+1)} = \arg \min_{\boldsymbol{\varepsilon}} \beta g(\boldsymbol{\varepsilon}) + Tr \left(\left(\mathbf{R}_2^{(t)} \right)^T (\mathbf{X} - \mathbf{XS}^{(t)} - \boldsymbol{\varepsilon}) \right) \\ + \frac{\mu_2}{2} \left\| \mathbf{X} - \mathbf{XS}^{(t)} - \boldsymbol{\varepsilon} \right\|_F^2. \end{aligned} \quad (3)$$

Define the proximal operator as

$$prox_{\lambda g}(\mathbf{Y}) := \arg \min_{\mathbf{X}} g(\mathbf{X}) + \frac{1}{2\lambda} \left\| \mathbf{X} - \mathbf{Y} \right\|_F^2. \quad (4)$$

We have that $\boldsymbol{\varepsilon}^{(t+1)}$ can be obtained by

$$\boldsymbol{\varepsilon}^{(t+1)} = prox_{\frac{\beta}{\mu_2} g} \left(\mathbf{Q}^{(t)} \right), \quad (5)$$

where $\mathbf{Q}^{(t)} = \mathbf{X} - \mathbf{XS}^{(t)} + \frac{\mathbf{R}_2^{(t)}}{\mu_2}$. According to different regularization strategies, $\boldsymbol{\varepsilon}^{(t+1)}$ can be updated with different closed-form solutions of (5). When we select the squared Frobenius norm $g(\boldsymbol{\varepsilon}) = \left\| \boldsymbol{\varepsilon} \right\|_F^2$, the $\boldsymbol{\varepsilon}^{(t+1)}$ can be computed by

$$\boldsymbol{\varepsilon}^{(t+1)} = \frac{\mathbf{Q}^{(t)}}{1 + 2\beta/\mu_2}. \quad (6)$$

When we select the ℓ_1 -norm $g(\boldsymbol{\varepsilon}) = \left\| \boldsymbol{\varepsilon} \right\|_1$, the $\boldsymbol{\varepsilon}^{(t+1)}$ can be updated as

$$\boldsymbol{\varepsilon}^{(t+1)} = shrink \left\{ \mathbf{Q}^{(t)}, \frac{\beta}{\mu_2} \right\}, \quad (7)$$

where $shrink\{\mathbf{X}, \lambda\}$ is an element-wise soft shrinkage operator defined as

$$[shrink\{\mathbf{X}, \lambda\}]_{i,j} = sign(x_{i,j}) \max\{|x_{i,j}| - \lambda, 0\}. \quad (8)$$

When we select the $\ell_{2,1}$ -norm $g(\boldsymbol{\varepsilon}) = \left\| \boldsymbol{\varepsilon} \right\|_{2,1}$, we can update $\boldsymbol{\varepsilon}^{(t+1)}$ by using the Lemma 3.3 of [1]

$$\boldsymbol{\varepsilon}_i^{(t+1)} = \max \left\{ \left\| \mathbf{Q}_i^{(t)} \right\|_2 - \frac{\beta}{\mu_2}, 0 \right\} \frac{\mathbf{Q}_i^{(t)}}{\left\| \mathbf{Q}_i^{(t)} \right\|_2}, \quad (9)$$

where we follow the convention $0 \cdot (0/0) = 0$.

\mathbf{S} -subproblem: with the fixed points $(\boldsymbol{\varepsilon}^{(t+1)}, \mathbf{W}^{(t)}, \mathbf{R}_1^{(t)}, \mathbf{R}_2^{(t)})$, we can update $\mathbf{S}^{(t+1)}$ by taking derivative of $L(\boldsymbol{\varepsilon}, \mathbf{S}, \mathbf{W}, \mathbf{R}_1, \mathbf{R}_2)$ with respect to \mathbf{S} with the unrelated term fixed and setting it to zero, then we obtain

$$\begin{aligned} \mathbf{S}^{(t+1)} = \arg \min_{\mathbf{S}} -Tr \left(\left(\mathbf{R}_1^{(t)} \right)^T \mathbf{S} \right) - Tr \left(\left(\mathbf{R}_2^{(t)} \right)^T \mathbf{XS} \right) \\ + \frac{\mu_1}{2} \left\| \mathbf{W}^{(t)} - \mathbf{S} \right\|_F^2 + \frac{\mu_2}{2} \left\| \mathbf{X} - \mathbf{XS} - \boldsymbol{\varepsilon}^{(t+1)} \right\|_F^2 \\ = \left(\mathbf{I}_{N_S} + \frac{\mu_2}{\mu_1} \mathbf{X}^T \mathbf{X} \right)^{-1} \boldsymbol{\Phi}^{(t+1)}, \end{aligned} \quad (10)$$

where $\Phi^{(t+1)} = \mathbf{W}^{(t)} + \frac{\mu_2 \mathbf{X}^T (\mathbf{X} - \epsilon^{(t+1)})}{\mu_1} + \frac{\mathbf{R}_1^{(t)} + \mathbf{X}^T \mathbf{R}_2^{(t)}}{\mu_1}$.

W-subproblem: with the fixed points $(\epsilon^{(t+1)}, \mathbf{S}^{(t+1)}, \mathbf{R}_1^{(t)}, \mathbf{R}_2^{(t)})$, the minimization of (2) with respect to \mathbf{W} can be formulated as

$$\begin{aligned} \mathbf{W}_i^{(t+1)} = \arg \min_{\mathbf{W}_i} & \left(\mathbf{D}_i^x + \mathbf{R}_{1i}^{(t)} \right)^T \mathbf{W}_i + \alpha_i \|\mathbf{W}_i\|_2^2 \\ & + \frac{\mu_1}{2} \left\| \mathbf{W}_i - \mathbf{S}_i^{(t+1)} \right\|_2^2 \\ \text{s.t. } & \mathbf{W}_i > 0, \quad \mathbf{W}_i^T \mathbf{1}_{N_S} = 1, \end{aligned} \quad (11)$$

where $\mathbf{R}_{1i}^{(t)}$ is the i -th column of $\mathbf{R}_1^{(t)}$. By defining $\gamma_i = \frac{\mu_1}{2} + \alpha_i$ and $\mathbf{P}_i = \mathbf{D}_i^x + \mathbf{R}_{1i}^{(t)} - \mu_1 \mathbf{S}_i^{(t+1)}$, the Lagrangian function of (11) is

$$\begin{aligned} \mathcal{L}(\mathbf{W}_i, \varsigma, \mathbf{v}) = & \gamma_i \|\mathbf{W}_i\|_2^2 + \mathbf{P}_i^T \mathbf{W}_i \\ & - \varsigma \left(\mathbf{W}_i^T \mathbf{1}_{N_S} - 1 \right) - \mathbf{v}^T \mathbf{W}_i, \end{aligned} \quad (12)$$

where $\varsigma \in \mathbb{R}$ and $\mathbf{v} \in \mathbb{R}^{N_S}$ are two Lagrangian multipliers. By using the Karush-Kuhn-Tucker (KKT) condition, the closed-form solution of $\mathbf{W}_i^{(t+1)}$ is

$$\mathbf{W}_i^{(t+1)} = \left(\frac{-\mathbf{P}_i + \varsigma}{2\gamma_i} \right)_+, \quad (13)$$

where the operator $(\mathbf{X})_+$ turns negative elements in \mathbf{X} to zero while keep the rest. Then, we can find that $\mathbf{W}_i^{(t+1)}$ is a sparse vector. We assume that $\mathbf{W}_i^{(t+1)}$ have k_i nonzero elements, i.e., only k_i neighbors have a connection with $\tilde{\mathbf{X}}_i$ with probabilities $\mathbf{W}_i^{(t+1)}$. We sort \mathbf{P}_i in ascending order denoted as $P_{(1),i}, P_{(2),i}, \dots, P_{(N_S),i}$. Then, the following inequalities hold

$$\begin{cases} \frac{-P_{(k_i),i} + \varsigma}{2\gamma_i} > 0 \\ \frac{-P_{(k_i+1),i} + \varsigma}{2\gamma_i} \leq 0 \end{cases}. \quad (14)$$

Considering the constraint $\mathbf{W}_i^T \mathbf{1}_{N_S} = 1$, we have

$$\sum_{h=1}^{k_i} \frac{-P_{(h),i} + \varsigma}{2\gamma_i} = 1. \quad (15)$$

Substitute (15) into (14), we have

$$\begin{cases} \gamma_i > \frac{k_i}{2} P_{(k_i),i} - \frac{1}{2} \sum_{h=1}^{k_i} P_{(h),i} \\ \gamma_i \leq \frac{k_i}{2} P_{(k_i+1),i} - \frac{1}{2} \sum_{h=1}^{k_i} P_{(h),i} \end{cases}. \quad (16)$$

Then, we can find that the regularization parameter α_i can be replaced by number of neighbors k_i when we set

$$\alpha_i = \frac{k_i}{2} P_{(k_i+1),i} - \frac{1}{2} \sum_{h=1}^{k_i} P_{(h),i} - \frac{\mu_1}{2}. \quad (17)$$

Therefore, the tuning of parameter α_i becomes the tuning of k_i , which is more intuitive (it has explicit meaning) and easier (it is an integer). With the k_i , the $\mathbf{W}_i^{(t+1)}$ can be updated as

$$W_{(j),i}^{(t+1)} = \begin{cases} \frac{P_{(k_i+1),i} - P_{(j),i}}{k_i P_{(k_i+1),i} - \sum_{h=1}^{k_i} P_{(h),i}}, & j \leq k_i \\ 0, & j > k_i \end{cases}. \quad (18)$$

Multipliers: finally, the two Lagrangian multipliers can be updated as

$$\begin{aligned} \mathbf{R}_1^{(t+1)} &= \mathbf{R}_1^{(t)} + \mu_1 \left(\mathbf{W}^{(t+1)} - \mathbf{S}^{(t+1)} \right), \\ \mathbf{R}_2^{(t+1)} &= \mathbf{R}_2^{(t)} + \mu_2 \left(\mathbf{X} - \mathbf{X} \mathbf{S}^{(t+1)} - \epsilon^{(t+1)} \right). \end{aligned} \quad (19)$$

II. LOOP OF THE GRAPH G

Lemma 1. The constructed graph $G = (V, E, w)$ has a loop for each vertex, that is, $w_{i,i} > 0$ for $i = 1, \dots, N_S$.

Proof: Assume by contradiction that there exists such optimal \mathbf{W}^* which has at least one diagonal element of 0. Without loss of generality, we assume that $w_{i,i}^* = 0$. By the definition, \mathbf{W}^* is the optimal solution of the following minimization problem

$$\begin{aligned} \min_{\mathbf{W}} & \sum_{i=1}^{N_S} \sum_{j=1}^{N_S} \|\mathbf{X}_i - \mathbf{X}_j\|_2^2 w_{i,j} + \sum_{i=1}^{N_S} \alpha_i \|\mathbf{W}_i\|_2^2 + \beta g(\epsilon) \\ \text{s.t. } & 0 \leq w_{i,j} \leq 1, \quad \sum_{i=1}^N w_{i,j} = 1, \quad \mathbf{X} = \mathbf{X} \mathbf{W} + \epsilon, \end{aligned} \quad (20)$$

where $\alpha_i, \beta > 0$ are the balancing parameters, and $g(\epsilon)$ represents the penalty term, which can be the $g(\epsilon) = \|\epsilon\|_F^2$, $\|\epsilon\|_1$, or $\|\epsilon\|_{2,1}$. Due to the columnwise independence property of \mathbf{W} in (20), we have that \mathbf{W}_i^* is the optimal solution of the following problem

$$\begin{aligned} \min_{\mathbf{W}_i} & \mathbf{D}_i^T \mathbf{W}_i + \alpha_i \|\mathbf{W}_i\|_2^2 + \beta g(\epsilon_i) \\ \text{s.t. } & 0 \leq w_{j,i} \leq 1, \quad \sum_{i=1}^N w_{j,i} = 1, \quad \mathbf{X}_i = \mathbf{X} \mathbf{W}_i + \epsilon_i, \end{aligned} \quad (21)$$

where \mathbf{D}_i is a distance vector with j -th element being $d_{j,i} = \|\mathbf{X}_i - \mathbf{X}_j\|_2^2$. Denote the objective function of (21) as

$$\Phi(\mathbf{W}_i) = \mathbf{D}_i^T \mathbf{W}_i + \alpha_i \|\mathbf{W}_i\|_2^2 + \beta g(\epsilon_i). \quad (22)$$

First, we construct a new $\bar{\mathbf{W}}_i$ as

$$\bar{w}_{j,i} = \begin{cases} \delta w_{j,i}^*, & \text{if } j \neq i \\ 1 - \delta, & \text{if } j = i \end{cases}, \quad (23)$$

with

$$\delta = \frac{1 - \|\mathbf{W}_i^*\|_2^2}{1 + \|\mathbf{W}_i^*\|_2^2} + \zeta, \quad (24)$$

and ζ is an arbitrary positive constant that satisfies $\zeta \in \left(0, \frac{2\|\mathbf{W}_i^*\|_2^2}{1 + \|\mathbf{W}_i^*\|_2^2}\right)$, which can enable $\frac{1 - \|\mathbf{W}_i^*\|_2^2}{1 + \|\mathbf{W}_i^*\|_2^2} < \delta < 1$. Then we have $0 \leq \bar{w}_{j,i} \leq 1$ and

$$\sum_{j=1}^{N_S} \bar{w}_{j,i} = \bar{w}_{i,i} + \sum_{j \neq i} \delta w_{j,i}^* = 1 - \delta + \sum_{j=1}^{N_S} \delta w_{j,i}^* = 1, \quad (25a)$$

$$\begin{aligned} \mathbf{D}_i^T \bar{\mathbf{W}}_i &= \sum_{j=1}^{N_S} \|\mathbf{X}_i - \mathbf{X}_j\|_2^2 \bar{w}_{j,i} = \sum_{j \neq i} \delta \|\mathbf{X}_i - \mathbf{X}_j\|_2^2 w_{j,i}^* \\ &= \delta \mathbf{D}_i^T \mathbf{W}_i^*, \end{aligned} \quad (25b)$$

$$\|\bar{\mathbf{W}}_i\|_2^2 = \bar{w}_{i,i}^2 + \sum_{j \neq i} (\delta w_{j,i}^*)^2 = (1 - \delta)^2 + \delta^2 \|\mathbf{W}_i^*\|_2^2, \quad (25c)$$

$$\begin{aligned} \bar{\boldsymbol{\varepsilon}}_i &= \mathbf{X}_i - \mathbf{X} \bar{\mathbf{W}}_i = \mathbf{X}_i - \mathbf{X}_i \bar{w}_{i,i} - \sum_{j \neq i} \delta \mathbf{X}_j w_{j,i}^* \\ &= \delta \left(\mathbf{X}_i - \sum_{j=1}^{N_S} \mathbf{X}_j w_{j,i}^* \right) = \delta \boldsymbol{\varepsilon}_i^*. \end{aligned} \quad (25d)$$

Substitute (25) into (22), we have

$$\begin{aligned} \Phi(\bar{\mathbf{W}}_i) &= \delta \mathbf{D}_i^T \mathbf{W}_i^* + \alpha_i \left((1 - \delta)^2 + \delta^2 \|\mathbf{W}_i^*\|_2^2 \right) \\ &\quad + \beta g(\delta \boldsymbol{\varepsilon}_i^*). \end{aligned} \quad (26)$$

Then, we have

$$\begin{aligned} \Phi(\mathbf{W}_i^*) - \Phi(\bar{\mathbf{W}}_i) &= (1 - \delta) \mathbf{D}_i^T \mathbf{W}_i^* + \beta (g(\boldsymbol{\varepsilon}_i^*) - g(\delta \boldsymbol{\varepsilon}_i^*)) \\ &\quad + \alpha_i \left((1 - \delta^2) \|\bar{\mathbf{W}}_i\|_2^2 - (1 - \delta)^2 \right) \\ &= (1 - \delta) \mathbf{D}_i^T \mathbf{W}_i^* + \beta (g(\boldsymbol{\varepsilon}_i^*) - g(\delta \boldsymbol{\varepsilon}_i^*)) \\ &\quad + \alpha_i (1 - \delta) \left(\delta \left(1 + \|\mathbf{W}_i^*\|_2^2 \right) - \left(1 - \|\mathbf{W}_i^*\|_2^2 \right) \right) \\ &\geq \alpha_i (1 - \delta) \left(\delta \left(1 + \|\mathbf{W}_i^*\|_2^2 \right) - \left(1 - \|\mathbf{W}_i^*\|_2^2 \right) \right) \\ &> 0, \end{aligned} \quad (27)$$

where the first inequality comes from $\mathbf{D}_i^T \mathbf{W}_i^* \geq 0$ and $g(\boldsymbol{\varepsilon}_i^*) \geq g(\delta \boldsymbol{\varepsilon}_i^*)$, and the second inequality comes from (24). Then, we have $\Phi(\mathbf{W}_i^*) > \Phi(\bar{\mathbf{W}}_i)$, which contradicts the optimality of \mathbf{W}_i^* . Then, we have $w_{i,i}^* > 0$. This completes the proof. ■

III. REFORMULATION OF THE HGLR

Reformulate the HGLR as follows:

$$\begin{aligned} &\sum_{e \in E^h} \sum_{\{\tilde{\mathbf{X}}_i, \tilde{\mathbf{X}}_j\} \in e} \frac{w^h(e) \tilde{h}(\tilde{\mathbf{X}}_i, e) \tilde{h}(\tilde{\mathbf{X}}_j, e)}{\delta(e)} \|\mathbf{Z}_i - \mathbf{Z}_j\|_2^2 \\ &= \sum_{\tilde{\mathbf{X}}_i \in V^h} \mathbf{Z}_i^T \mathbf{Z}_i \sum_{e \in E^h} w^h(e) \tilde{h}(\tilde{\mathbf{X}}_i, e) \sum_{\tilde{\mathbf{X}}_j \in V^h} \frac{\tilde{h}(\tilde{\mathbf{X}}_j, e)}{\delta(e)} \\ &\quad + \sum_{\tilde{\mathbf{X}}_j \in V^h} \mathbf{Z}_j^T \mathbf{Z}_j \sum_{e \in E^h} w^h(e) \tilde{h}(\tilde{\mathbf{X}}_j, e) \sum_{\tilde{\mathbf{X}}_i \in V^h} \frac{\tilde{h}(\tilde{\mathbf{X}}_i, e)}{\delta(e)} \\ &\quad - \sum_{e \in E^h} \sum_{\tilde{\mathbf{X}}_i, \tilde{\mathbf{X}}_j \in V^h} 2 \mathbf{Z}_i^T \frac{w^h(e) \tilde{h}(\tilde{\mathbf{X}}_i, e) \tilde{h}(\tilde{\mathbf{X}}_j, e)}{\delta(e)} \mathbf{Z}_j. \end{aligned} \quad (28)$$

Substitute the definitions of $d(v) = \sum_{e \in E^h} w^h(e) h(v, e)$, $\delta(e) = \sum_{v \in V^h} h(v, e)$ into (28), we have

$$\begin{aligned} &\sum_{e \in E^h} \sum_{\{\tilde{\mathbf{X}}_i, \tilde{\mathbf{X}}_j\} \in e} \frac{w^h(e) \tilde{h}(\tilde{\mathbf{X}}_i, e) \tilde{h}(\tilde{\mathbf{X}}_j, e)}{\delta(e)} \|\mathbf{Z}_i - \mathbf{Z}_j\|_2^2 \\ &= 2Tr \left(\mathbf{Z} \mathbf{D}_v \mathbf{Z}^T \right) - 2Tr \left(\mathbf{Z} \tilde{\mathbf{H}} \mathbf{W}^h \mathbf{D}_e^{-1} \tilde{\mathbf{H}}^T \mathbf{Z}^T \right) \\ &= 2Tr \left(\mathbf{Z} \mathbf{L}^h \mathbf{Z}^T \right), \end{aligned} \quad (29)$$

where the last equation comes from the definition of hypergraph Laplacian matrix as $\mathbf{L}^h = \mathbf{D}_v - \tilde{\mathbf{H}} \mathbf{W}^h \mathbf{D}_e^{-1} \tilde{\mathbf{H}}^T$.

REFERENCES

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