Supplementary Materials Localized Lasso for High-Dimensional Regression

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Propositions used for deriving Eq. (4) in main paper

Proposition 1 Under $r_{ij} \geq 0$, $r_{ij} = r_{ji}$, $r_{ii} = 0$, we have

$$\frac{\partial}{\partial \text{vec}(\boldsymbol{W})} \sum_{i,j=1}^{n} r_{ij} \|\boldsymbol{w}_i - \boldsymbol{w}_j\|_2 = 2\boldsymbol{F}_g \text{vec}(\boldsymbol{W}),$$

where

$$\begin{aligned} \boldsymbol{F}_g &= \boldsymbol{I}_d \otimes \boldsymbol{C}, \\ [\boldsymbol{C}]_{i,j} &= \left\{ \begin{array}{ll} \sum_{j'=1}^n \frac{r_{ij'}}{\|\boldsymbol{w}_i - \boldsymbol{w}_j'\|_2} - \frac{r_{ij}}{\|\boldsymbol{w}_i - \boldsymbol{w}_j\|_2} & (i = j) \\ \frac{-r_{ij}}{\|\boldsymbol{w}_i - \boldsymbol{w}_i\|_2} & (i \neq j) \end{array} \right.. \end{aligned}$$

Proof: Under $r_{ij} \ge 0$, $r_{ij} = r_{ji}$, $r_{ii} = 0$, the derivative of the network regularization term with respect to \mathbf{w}_k is given as

$$\frac{\partial}{\partial \boldsymbol{w}_{k}} \sum_{i,j=1}^{n} r_{ij} \| \boldsymbol{w}_{i} - \boldsymbol{w}_{j} \|_{2} = \sum_{i=1}^{n} r_{ik} \frac{\boldsymbol{w}_{k} - \boldsymbol{w}_{i}}{\| \boldsymbol{w}_{k} - \boldsymbol{w}_{i} \|_{2}} + \sum_{j=1}^{n} r_{kj} \frac{\boldsymbol{w}_{k} - \boldsymbol{w}_{j}}{\| \boldsymbol{w}_{j} - \boldsymbol{w}_{k} \|_{2}}$$

$$= \boldsymbol{w}_{k} \left(\sum_{i=1}^{n} \frac{r_{ik}}{\| \boldsymbol{w}_{k} - \boldsymbol{w}_{i} \|_{2}} + \sum_{j=1}^{n} \frac{r_{kj}}{\| \boldsymbol{w}_{j} - \boldsymbol{w}_{k} \|_{2}} \right)$$

$$- \sum_{i=1}^{n} \frac{r_{ik}}{\| \boldsymbol{w}_{k} - \boldsymbol{w}_{i} \|_{2}} \boldsymbol{w}_{i} - \sum_{j=1}^{n} \frac{r_{kj}}{\| \boldsymbol{w}_{j} - \boldsymbol{w}_{k} \|_{2}} \boldsymbol{w}_{j}$$

$$= 2 \left(\boldsymbol{w}_{k} \sum_{i=1}^{n} \frac{r_{ik}}{\| \boldsymbol{w}_{k} - \boldsymbol{w}_{i} \|_{2}} - \sum_{i=1}^{n} \frac{r_{ik}}{\| \boldsymbol{w}_{k} - \boldsymbol{w}_{i} \|_{2}} \boldsymbol{w}_{i} \right).$$

Thus,

$$\frac{\partial}{\partial \boldsymbol{W}} \sum_{i,j=1}^{n} r_{ij} \|\boldsymbol{w}_i - \boldsymbol{w}_j\|_2 = 2\boldsymbol{C}\boldsymbol{W},$$

where $\mathbf{W} = [\mathbf{w}_1, \dots, \mathbf{w}_n]^{\top} \in \mathbb{R}^{n \times d}$. Since $\text{vec}(\mathbf{CW} \mathbf{I}_d) = (\mathbf{I}_d \otimes \mathbf{C}) \text{vec}(\mathbf{W})$, we have

$$\frac{\partial}{\partial \text{vec}(\boldsymbol{W})} \sum_{i,j=1}^{n} r_{ij} \|\boldsymbol{w}_i - \boldsymbol{w}_j\|_2 = 2(\boldsymbol{I}_d \otimes \boldsymbol{C}) \text{vec}(\boldsymbol{W}),$$

where $I_d \in \mathbb{R}^{d \times d}$ is the identity matrix and $\text{vec}(\cdot)$ is the vectorization operator.

Proposition 2

$$\frac{\partial}{\partial \text{vec}(\boldsymbol{W})} \sum_{i=1}^{n} \|\boldsymbol{w}_i\|_1^2 = 2\boldsymbol{F}_e \text{vec}(\boldsymbol{W}),$$

where

$$[\boldsymbol{F}_e]_{\ell,\ell} = \sum_{i=1}^n rac{I_{i,\ell} \| \boldsymbol{w}_i \|_1}{[\operatorname{vec}(|\boldsymbol{W}|)]_\ell}.$$

Hence, $I_{i,\ell} \in \{0, 1\}$ are the group index indicators: $I_{i,\ell} = 1$ if the ℓ -th element $[\text{vec}(\boldsymbol{W})]_{\ell}$ belongs to group i (i.e., $[\text{vec}(\boldsymbol{W})]_{\ell}$ is the element of \boldsymbol{w}_i), otherwise $I_{i,\ell} = 0$.

Propositions and lemmas used for deriving Theorem 1 in main paper

Proposition 3 Under $r_{ij} \geq 0$, $r_{ij} = r_{ji}$, $r_{ii} = 0$, we have

$$vec(\boldsymbol{W})^{\top} \boldsymbol{F}_{g}^{(t)} vec(\boldsymbol{W}) = \sum_{i,j=1}^{n} r_{ij} \frac{\|\boldsymbol{w}_{i} - \boldsymbol{w}_{j}\|_{2}^{2}}{2\|\boldsymbol{w}_{i}^{(t)} - \boldsymbol{w}_{i}^{(t)}\|_{2}},$$

where

$$F_g^{(t)} = I_d \otimes C^{(t)},$$

$$[C^{(t)}]_{i,j} = \begin{cases} \sum_{j'=1}^{n} \frac{r_{ij'}}{\|\boldsymbol{w}_i^{(t)} - \boldsymbol{w}_{j'}^{(t)}\|_2} - \frac{r_{ij}}{\|\boldsymbol{w}_i^{(t)} - \boldsymbol{w}_{j}^{(t)}\|_2} & (i = j) \\ \frac{-r_{ij}}{\|\boldsymbol{w}_i^{(t)} - \boldsymbol{w}_j^{(t)}\|_2} & (i \neq j) \end{cases}.$$

Proof:

$$\begin{split} & \sum_{i,j=1}^{n} r_{ij} \frac{\|\boldsymbol{w}_{i} - \boldsymbol{w}_{j}\|_{2}^{2}}{2\|\boldsymbol{w}_{i}^{(t)} - \boldsymbol{w}_{j}^{(t)}\|_{2}} \\ & = \sum_{i=1}^{n} \boldsymbol{w}_{i}^{\top} \boldsymbol{w}_{i} \sum_{j=1}^{n} \frac{r_{ij}}{2\|\boldsymbol{w}_{i}^{(t)} - \boldsymbol{w}_{j}^{(t)}\|_{2}} + \sum_{j=1}^{n} \boldsymbol{w}_{j}^{\top} \boldsymbol{w}_{j} \sum_{i=1}^{n} \frac{r_{ij}}{2\|\boldsymbol{w}_{i}^{(t)} - \boldsymbol{w}_{j}^{(t)}\|_{2}} - 2 \sum_{i=1}^{n} \sum_{j=1}^{n} \boldsymbol{w}_{i}^{\top} \boldsymbol{w}_{j} \frac{r_{ij}}{2\|\boldsymbol{w}_{i}^{(t)} - \boldsymbol{w}_{j}^{(t)}\|_{2}} \\ & = \operatorname{tr}(\boldsymbol{W}^{\top} \boldsymbol{C}^{(t)} \boldsymbol{W}) \\ & = \operatorname{vec}(\boldsymbol{W})^{\top} (\boldsymbol{I}_{d} \otimes \boldsymbol{C}^{(t)}) \operatorname{vec}(\boldsymbol{W}), \end{split}$$

where $I_d \in \mathbb{R}^{d \times d}$ is the identity matrix, $tr(\cdot)$ is the trace operator, and $vec(\cdot)$ is the vectorization operator.

Lemma 4 Under the updating rule of Eq. (6).

$$\widetilde{J}(\boldsymbol{W}^{(t+1)}) - \widetilde{J}(\boldsymbol{W}^{(t)}) \le 0.$$

Proof: Under the updating rule of Eq. (6), since Eq.(5) is a convex function and the optimal solution is obtained by solving $\frac{\partial \widetilde{J}(\mathbf{W})}{\partial \mathbf{W})} = 0$, the obtained solution $\mathbf{W}^{(t+1)}$ is the global solution. That is, $\widetilde{J}(\mathbf{W}^{(t+1)}) \leq \widetilde{J}(\mathbf{W}^{(t)})$.

Lemma 5 For any nonzero vectors $\mathbf{w}, \mathbf{w}^{(t)} \in \mathbb{R}^d$, the following inequality holds Nie et al. [2010]:

$$\| \boldsymbol{w} \|_2 - \frac{\| \boldsymbol{w} \|_2^2}{2 \| \boldsymbol{w}^{(t)} \|_2} \le \| \boldsymbol{w}^{(t)} \|_2 - \frac{\| \boldsymbol{w}^{(t)} \|_2^2}{2 \| \boldsymbol{w}^{(t)} \|_2}.$$

 $\textbf{Lemma 6} \ \textit{For} \ r_{i,j} \geq 0, \forall i,j, \ \textit{the following inequality holds for any non-zero vectors} \ \boldsymbol{w}_i^{(t)} - \boldsymbol{w}_j^{(t)}, \boldsymbol{w}_i^{(t+1)} - \boldsymbol{w}_j^{(t+1)} = \boldsymbol{w}_j^{(t+1)} + \boldsymbol{w}_j^{(t+1)} = \boldsymbol{w}_j$

$$\sum_{i,j=1}^{n} r_{ij} \| \boldsymbol{w}_{i}^{(t+1)} - \boldsymbol{w}_{j}^{(t+1)} \|_{2} - \text{vec}(\boldsymbol{W}^{(t+1)})^{\top} \boldsymbol{F}_{g}^{(t)} \text{vec}(\boldsymbol{W}^{(t+1)})$$
$$- \left(\sum_{i,j=1}^{n} r_{ij} \| \boldsymbol{w}_{i}^{(t)} - \boldsymbol{w}_{j}^{(t)} \|_{2} - \text{vec}(\boldsymbol{W}^{(t)})^{\top} \boldsymbol{F}_{g}^{(t)} \text{vec}(\boldsymbol{W}^{(t)}) \right) \leq 0.$$

Proof: $\operatorname{vec}(\boldsymbol{W})^{\top} \boldsymbol{F}_g^{(t)} \operatorname{vec}(\boldsymbol{W})$ can be written as

$$vec(\boldsymbol{W})^{\top} \boldsymbol{F}_{g}^{(t)} vec(\boldsymbol{W}) = \sum_{i,j=1}^{n} r_{ij} \frac{\|\boldsymbol{w}_{i} - \boldsymbol{w}_{j}\|_{2}^{2}}{2\|\boldsymbol{w}_{i}^{(t)} - \boldsymbol{w}_{i}^{(t)}\|_{2}}.$$

where $r_{ij} \geq 0$.

Then, the left hand side equation can be written as

$$\Delta_g = \sum_{i,j=1}^n r_{ij} \left(\| \boldsymbol{w}_i^{(t+1)} - \boldsymbol{w}_j^{(t+1)} \|_2 - \frac{\| \boldsymbol{w}_i^{(t+1)} - \boldsymbol{w}_j^{(t+1)} \|_2^2}{2 \| \boldsymbol{w}_i^{(t)} - \boldsymbol{w}_j^{(t)} \|_2} \right) - \sum_{i,j=1}^n r_{ij} \left(\| \boldsymbol{w}_i^{(t)} - \boldsymbol{w}_j^{(t)} \|_2 - \frac{\| \boldsymbol{w}_i^{(t)} - \boldsymbol{w}_j^{(t)} \|_2^2}{2 \| \boldsymbol{w}_i^{(t)} - \boldsymbol{w}_j^{(t)} \|_2} \right).$$

Using Lemma 5, $\Delta_g \leq 0$.

Lemma 7 The following inequality holds for any non-zero vectors Kong et al. [2014]:

$$\sum_{i=1}^{n} \|\boldsymbol{w}_{i}^{(t+1)}\|_{1}^{2} - \text{vec}(\boldsymbol{W}^{(t+1)})^{\top} \boldsymbol{F}_{e}^{(t)} \text{vec}(\boldsymbol{W}^{(t+1)})$$
$$-\left(\sum_{i=1}^{n} \|\boldsymbol{w}_{i}^{(t)}\|_{1}^{2} - \text{vec}(\boldsymbol{W}^{(t)})^{\top} \boldsymbol{F}_{e}^{(t)} \text{vec}(\boldsymbol{W}^{(t)})\right) \leq 0.$$
(1)

Proof: $\operatorname{vec}(\boldsymbol{W})^{\top} \boldsymbol{F}_{e}^{(t)} \operatorname{vec}(\boldsymbol{W})$ can be written as

$$\begin{aligned} \text{vec}(\boldsymbol{W})^{\top} \boldsymbol{F}_{e}^{(t)} \text{vec}(\boldsymbol{W}) &= \sum_{\ell=1}^{dn} [\text{vec}(\boldsymbol{W})]_{\ell}^{2} \sum_{i=1}^{n} \frac{I_{i,\ell} \|\boldsymbol{w}_{i}^{(t)}\|_{1}}{[\text{vec}(|\boldsymbol{W}^{(t)}|)]_{\ell}} \\ &= \sum_{i=1}^{n} \left(\sum_{j=1}^{d} \frac{[\boldsymbol{w}_{i}]_{j}^{2}}{[|\boldsymbol{w}_{i}^{(t)}|]_{j}} \right) \|\boldsymbol{w}_{i}^{(t)}\|_{1}. \end{aligned}$$

Thus, the left hand equation is written as

$$\Delta_e = \sum_{i=1}^n \left[\left(\sum_{j=1}^d [\boldsymbol{w}_i^{(t+1)}]_j \right)^2 - \left(\sum_{j=1}^d \frac{[\boldsymbol{w}_i^{(t+1)}]_j^2}{[|\boldsymbol{w}_i^{(t)}|]_j} \right) \left(\sum_{j=1}^d [\boldsymbol{w}_i^{(t)}]_j \right) \right]$$

$$= \sum_{i=1}^n \left[\left(\sum_{j=1}^d a_j^{(t)} b_j^{(t)} \right)^2 - \left(\sum_{j=1}^d (a_j^{(t)})^2 \right) \left(\sum_{j=1}^d (b_j^{(t)})^2 \right) \right] \le 0,$$

where $a_j^{(t)} = \frac{[|\boldsymbol{w}_i^{(t+1)}|]_j}{\sqrt{[|\boldsymbol{w}_i^{(t)}|]_j}}$ and $b_j^{(t)} = \sqrt{[|\boldsymbol{w}_i^{(t)}|]_j}$, and $\text{vec}(\boldsymbol{W}^{(t)})^{\top} \boldsymbol{F}_e^{(t)} \text{vec}(\boldsymbol{W}^{(t)}) = \sum_{i=1}^n \|\boldsymbol{w}_i^{(t)}\|_1^2$. The inequality holds due to cauchy inequality Steele [2004].

 $\textbf{Lemma 8} \ \textit{For } r_{i,j} \geq 0, \forall i,j, \ \textit{the following inequality holds for any non-zero vectors } \boldsymbol{w}_i^{(t)} - \boldsymbol{w}_j^{(t)}, \boldsymbol{w}_i^{(t+1)} - \boldsymbol{w}_j^{(t+1)} : \boldsymbol{w}_j^{(t+1)} = \boldsymbol{w}_j^{$

$$J(\mathbf{W}^{(t+1)}) - J(\mathbf{W}^{(t)}) \le \widetilde{J}(\mathbf{W}^{(t+1)}) - \widetilde{J}(\mathbf{W}^{(t)}).$$

Proof: The difference between the right and left side equations is given as

$$\Delta = J(\boldsymbol{W}^{(t+1)}) - J(\boldsymbol{W}^{(t)}) - (\widetilde{J}(\boldsymbol{W}^{(t+1)}) - \widetilde{J}(\boldsymbol{W}^{(t)}))$$

$$= \lambda_1 \left(\sum_{i,j=1}^n r_{ij} \| \boldsymbol{w}_i^{(t+1)} - \boldsymbol{w}_j^{(t+1)} \|_2 - \text{vec}(\boldsymbol{W}^{(t+1)})^\top \boldsymbol{F}_g^{(t)} \text{vec}(\boldsymbol{W}^{(t+1)}) \right)$$

$$- \left[\sum_{i,j=1}^n r_{ij} \| \boldsymbol{w}_i^{(t)} - \boldsymbol{w}_j^{(t)} \|_2 - \text{vec}(\boldsymbol{W}^{(t)})^\top \boldsymbol{F}_g^{(t)} \text{vec}(\boldsymbol{W}^{(t)}) \right] \right)$$

$$+ \lambda_2 \left(\sum_{i=1}^n \| \boldsymbol{w}_i^{(t+1)} \|_1^2 - \text{vec}(\boldsymbol{W}^{(t+1)})^\top \boldsymbol{F}_e^{(t)} \text{vec}(\boldsymbol{W}^{(t+1)}) \right)$$

$$- \left[\sum_{i=1}^n \| \boldsymbol{w}_i^{(t)} \|_1^2 - \text{vec}(\boldsymbol{W}^{(t)})^\top \boldsymbol{F}_e^{(t)} \text{vec}(\boldsymbol{W}^{(t)}) \right] \right)$$

Based on Lemma 6 and 7, $\Delta \leq 0$.

References

Deguang Kong, Ryohei Fujimaki, Ji Liu, Feiping Nie, and Chris Ding. Exclusive feature learning on arbitrary structures via ℓ_{12} -norm. In NIPS, 2014.

Feiping Nie, Heng Huang, Xiao Cai, and Chris H Ding. Efficient and robust feature selection via joint $\ell_{2,1}$ -norms minimization. In NIPS, 2010.

J Michael Steele. An introduction to the art of mathematical inequalities: The Cauchy-Schwarz master class, 2004.