Supplementary Materials for "Exploring Latent Sparse Graph for Large-Scale Semi-supervised Learning"

Zitong Wang[1], Li Wang✉[2,3], Raymond Chan[4], and Tieyong Zeng[5]

[1] Department of Industrial Engineering and Operations Research, Columbia University in the City of New York, USA. zw2690@columbia.edu
[2] Department of Computer Science and Engineering, University of Texas at Arlington, Arlington, TX 76019-0408, USA. li.wang@uta.edu
[3] Department of Mathematics, University of Texas at Arlington, Arlington, TX 76019-0408, USA.
[4] Department of Mathematics, City University of Hong Kong, Hong Kong. rchan.sci@cityu.edu.hk
[5] Department of Mathematics, The Chinese University of Hong Kong, Hong Kong. zeng@math.cuhk.edu.hk

A Proof of Proposition 1

Before we prove that the matrix W is symmetric, we need to show the following results.

Proposition 1 *Let $P \in \mathbb{R}^{(n+k)\times(n+k)}$, and suppose $(I_{n+k} - \alpha P)^{-1}$ exists. Then $P^2(I_{n+k} - \alpha P)^{-1} = (I_{n+k} - \alpha P)^{-1}P^2$.*

Proof. It always holds that

$$P^2(I_{n+k} - \alpha P) = (I_{n+k} - \alpha P)P^2 = P^2 - \alpha P^3. \tag{S1}$$

Since $(I_{n+k} - \alpha P)^{-1}$ exists, we multiply $(I_{n+k} - \alpha P)^{-1}$ on both sides of equation (S1) to get

$$(I_{n+k} - \alpha P)^{-1}P^2 = P^2(I_{n+k} - \alpha P)^{-1}. \tag{S2}$$

The proof is completed.

Lemma 1. *Let $P = \Gamma^{-1}Q$ be given by (26). The eigenvalues of P are real, and lie in $[-1, 1]$.*

Proof. By definition, we have $P \geq 0$ and $P\mathbf{1}_{n+k} = \mathbf{1}_{n+k}$. So, all elements in P are between 0 and 1. The row sums of P is 1. The characteristic polynomial of P is

$$\det(\lambda I_{n+k} - P) = \det\left(\Gamma^{-\frac{1}{2}}\left(\lambda I_{n+k} - \Gamma^{-\frac{1}{2}}Q\Gamma^{-\frac{1}{2}}\right)\Gamma^{\frac{1}{2}}\right).$$

The eigenvalues of P are the same as the eigenvalues of matrix $\Gamma^{-\frac{1}{2}}Q\Gamma^{-\frac{1}{2}}$. Matrix $\Gamma^{-\frac{1}{2}}Q\Gamma^{-\frac{1}{2}}$ is symmetric, so its eigenvalues are real, i.e., the eigenvalues of P are real. By the Gershgorin circle theorem [1], we conclude all the eigenvalues of P lie in $[-1, 1]$.

Now, we are ready to prove Proposition 1. Note $Q = Q^T$, $P = \Gamma^{-1}Q$, $P^T = Q\Gamma^{-1} = \Gamma P \Gamma^{-1}$. Since $P^2(I_{n+k} - \alpha P)^{-1} = (I_{n+k} - \alpha P)^{-1}P^2$ by Proposition 1, we have

$$\begin{aligned}(P^2(I-\alpha P)^{-1})^T &= (I_{n+k} - \alpha P^T)^{-1}(P^T)^2 \\ &= (I_{n+k} - \alpha \Gamma P \Gamma^{-1})^{-1}\Gamma P^2 \Gamma^{-1} \\ &= \left(\Gamma(I_{n+k} - \alpha P)\Gamma^{-1}\right)^{-1}\Gamma P^2\Gamma^{-1} \\ &= \Gamma(I_{n+k} - \alpha P)^{-1}P^2\Gamma^{-1} \\ &= \Gamma P^2(I_{n+k} - \alpha P)^{-1}\Gamma^{-1}.\end{aligned}$$

On the other hand, by (25) and (26), we get

$$(P^2(I-\alpha P)^{-1})^T = \begin{bmatrix} W & A_1 \\ A_2 & A_3 \end{bmatrix}^T = \begin{bmatrix} W^T & A_2^T \\ A_1^T & A_3^T \end{bmatrix}, \tag{S3}$$

and

$$\begin{aligned}\Gamma P^2(I-\alpha P)^{-1}\Gamma^{-1} &= \begin{bmatrix} I_n & 0 \\ 0 & E \end{bmatrix}\begin{bmatrix} W & A_1 \\ A_2 & A_3 \end{bmatrix}\begin{bmatrix} I_n & 0 \\ 0 & E^{-1} \end{bmatrix} \\ &= \begin{bmatrix} W & A_1E^{-1} \\ EA_2 & EA_3E^{-1} \end{bmatrix}.\end{aligned} \tag{S4}$$

Comparing these two matrices in (S3) and (S4), we have $W = W^T$, i.e., W is symmetric.

Since the spectrum of P lies in $[-1, 1]$, and $\alpha \in (0, 1)$, we have $(I_{n+k} - \alpha P)^{-1} = \sum_{t=0}^{\infty}(\alpha P)^t$, i.e., the right side matrix series converges. Then

$$P^2(I_{n+k} - \alpha P)^{-1} = P^2 + \alpha P^3 + \alpha^2 P^4 + \cdots. \tag{S5}$$

Since $P \geq 0$, every term on the right hand side is nonnegative, and $W \geq 0$. The proof is completed.

B Proof of Proposition 2

If either $\eta = 0$ or $G = 0$, we have

$$\begin{aligned}P &= \mathbf{diag}\left(\begin{bmatrix} \mathbf{0}_{n\times n} & Z \\ Z^T & \mathbf{0}_{k\times k} \end{bmatrix}\mathbf{1}_{n+k}\right)^{-1}\begin{bmatrix} \mathbf{0}_{n\times n} & Z \\ Z^T & \mathbf{0}_{k\times k} \end{bmatrix} \\ &= \mathbf{diag}\left(\begin{bmatrix} Z\mathbf{1}_k \\ Z^T\mathbf{1}_n \end{bmatrix}\right)^{-1}\begin{bmatrix} \mathbf{0}_{n\times n} & Z \\ Z^T & \mathbf{0}_{k\times k} \end{bmatrix} \\ &= \mathbf{diag}\left(\begin{bmatrix} \mathbf{1}_n \\ Z^T\mathbf{1}_n \end{bmatrix}\right)^{-1}\begin{bmatrix} \mathbf{0}_{n\times n} & Z \\ Z^T & \mathbf{0}_{k\times k} \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{I}_{n\times n} & \mathbf{0}_{n\times k} \\ \mathbf{0}_{k\times n} & \Lambda^{-1} \end{bmatrix}\begin{bmatrix} \mathbf{0}_{n\times n} & Z \\ Z^T & \mathbf{0}_{k\times k} \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{0}_{n\times n} & Z \\ \Lambda^{-1}Z^T & \mathbf{0}_{k\times k} \end{bmatrix},\end{aligned}$$

and

$$P^2 = \begin{bmatrix} \mathbf{0}_{n\times n} & Z \\ \Lambda^{-1}Z^T & \mathbf{0}_{k\times k} \end{bmatrix} \begin{bmatrix} \mathbf{0}_{n\times n} & Z \\ \Lambda^{-1}Z^T & \mathbf{0}_{k\times k} \end{bmatrix} = \begin{bmatrix} Z\Lambda^{-1}Z^T & \mathbf{0}_{n\times k} \\ \mathbf{0}_{k\times n} & \Lambda^{-1}Z^T Z \end{bmatrix},$$

where $\Lambda = \mathbf{diag}(Z^T \mathbf{1}_n)$. Since $\alpha = 0$ and by definition, we have

$$W = Z\Lambda^{-1}Z^T,$$

which is the same as W in AGR for a given Z.

C Proof of Proposition 3

Lemma 2. *For $\alpha \in (0, 1)$, the eigenvalues of matrix*

$$\widetilde{P} = \alpha\eta E^{-1}G + \alpha^2 E^{-1}Z^T Z \tag{S6}$$

are real and lie in $(-1, 1)$.

Proof. By the definition of E, G, Z, we have $\widetilde{P} \geq 0$. The characteristic polynomial of $\widetilde{P}$ is

$$\begin{aligned} &\det(\lambda I_k - \widetilde{P}) \\ =&\det\left(E^{-\frac{1}{2}}\left(\lambda I_k - E^{-\frac{1}{2}}(\alpha\eta G + \alpha^2 Z^T Z)E^{-\frac{1}{2}}\right)E^{\frac{1}{2}}\right). \end{aligned}$$

The eigenvalues of $\widetilde{P}$ are the same as the eigenvalues of $E^{-\frac{1}{2}}(\alpha\eta G + \alpha^2 Z^T Z)E^{-\frac{1}{2}}$. Since matrix $E^{-\frac{1}{2}}(\alpha\eta G + \alpha^2 Z^T Z)E^{-\frac{1}{2}}$ is symmetric, all its eigenvalues are real, i.e. the matrix $\widetilde{P}$ has only real eigenvalues. Now let us prove the row sums of $\widetilde{P}$ are bounded by 1.

$$\begin{aligned} \widetilde{P}\mathbf{1}_k &= \alpha\eta E^{-1}G\mathbf{1}_k + \alpha^2 E^{-1}Z^T Z\mathbf{1}_k \\ &= \alpha\eta E^{-1}G\mathbf{1}_k + \alpha^2 E^{-1}Z^T\mathbf{1}_n \\ &\leq \alpha E^{-1}(\eta G\mathbf{1}_k + Z^T\mathbf{1}_n) \quad (\text{since } \alpha \in (0,1)) \\ &= \alpha\mathbf{1}_k < \mathbf{1}_k. \end{aligned}$$

By the Gershgorin circle theorem [1], we have the eigenvalues of $\widetilde{P}$ lie in $(-1, 1)$. The proof is completed.

By the definition of matrix P and matrix inversion in a 2×2 block form, we have the following equations:

$$(I_{n+k} - \alpha P)^{-1} = \begin{bmatrix} I_n & -\alpha Z \\ -\alpha E^{-1}Z^T & I_k - \alpha\eta E^{-1}G \end{bmatrix}^{-1} = \begin{bmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{bmatrix}, \tag{S7}$$

where

$$\begin{aligned}
L_{11} &= I_n + \alpha^2 Z(I_k - \alpha\eta E^{-1}G - \alpha^2 E^{-1}Z^T Z)^{-1}E^{-1}Z^T, \\
L_{12} &= \alpha Z(I_k - \alpha\eta E^{-1}G - \alpha^2 E^{-1}Z^T Z)^{-1}, \\
L_{21} &= \alpha(I_k - \alpha\eta E^{-1}G - \alpha^2 E^{-1}Z^T Z)^{-1}E^{-1}Z^T, \\
L_{22} &= (I_k - \alpha\eta E^{-1}G - \alpha^2 E^{-1}Z^T Z)^{-1}.
\end{aligned}$$

It is worth noting that (S7) holds in the condition that matrix $I_k - \alpha\eta E^{-1}G - \alpha^2 E^{-1}Z^T Z$ must be invertible. The inversion is guaranteed by Lemma 2.

According to Lemma 2, it is clear that $I_k - \widetilde{P}$ has eigenvalues in $(0, 2)$, so (S7) holds for all $\alpha \in (0, 1)$. Accordingly, the right hand side of (8) is:

$$P^2(I_{n+k} - \alpha P)^{-1} = \begin{bmatrix} W & A_1 \\ A_2 & A_3 \end{bmatrix}, \tag{S8}$$

where

$$\begin{aligned}
W &= ZE^{-1}Z^T L_{11} + \eta Z E^{-1} G L_{21}, \qquad \text{(S9)} \\
A_1 &= ZE^{-1}Z^T L_{12} + \eta Z E^{-1} G L_{22}, \\
A_2 &= \eta E^{-1}GE^{-1}Z^T L_{11} + \left(E^{-1}Z^T Z + \eta^2 (E^{-1}G)^2\right) L_{21}, \\
A_3 &= \eta E^{-1}GE^{-1}Z^T L_{12} + \left(E^{-1}Z^T Z + \eta^2 (E^{-1}G)^2\right) L_{22}.
\end{aligned}$$

Substituting L_{11} and L_{21} into (S9), we achieve the goal.

References

1. Geršgorin, S.: Über die abgrenzung der eigenwerte einer matrix. Izv. Akad. Nauk SSSR Ser. Mat **1**(7), 749–755 (1931)