Supplementary Material for Bipartite Edge Prediction via Transductive Learning over Product Graphs

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A. Remarks

Before going through the proofs, we review some useful facts about the Kronecker (Tensor) product. Those properties are commonly used for solving Sylvester equations. More details can be found in *The Matrix Cookbook*.

Remark 1. $(\boldsymbol{AC}) \otimes (\boldsymbol{BD}) = (\boldsymbol{A} \otimes \boldsymbol{B})(\boldsymbol{C} \otimes \boldsymbol{D})$

Remark 2. $(\boldsymbol{A} \otimes \boldsymbol{B})^\top = \boldsymbol{A}^\top \otimes \boldsymbol{B}^\top$

Remark 3. $\text{vec}\left(\boldsymbol{BCA}^\top\right) = \left(\boldsymbol{B} \otimes \boldsymbol{A}\right)\text{vec}\left(\boldsymbol{C}\right)$ [1]

B. Spectral Graph Products

Let us verify that both the Tensor and Cartesian graph products are members of the Spectral Graph Product (SGP) family. For any graph $\mathcal{G}$, we use $\boldsymbol{\Lambda}_\mathcal{G}$ to denote the diagonal matrix consisting of the eigenvalues of its adjacency matrix $\boldsymbol{G}$.

B.1. Tensor Graph Product

Suppose $x \circ y = xy$. According to Definition 5, we have

$$[\boldsymbol{\Lambda}_{\mathcal{G}\circ\mathcal{H}}]_{(i,j),(i,j)} = [\lambda_\mathcal{G}]_i \circ [\lambda_\mathcal{H}]_j = [\lambda_\mathcal{G}]_i [\lambda_\mathcal{H}]_j \tag{1}$$

which implies $\boldsymbol{\Lambda}_{\mathcal{G}\circ\mathcal{H}} = \boldsymbol{\Lambda}_\mathcal{G} \otimes \boldsymbol{\Lambda}_\mathcal{H}$. Therefore

$$\begin{aligned}
\boldsymbol{G} \circ \boldsymbol{H} &= (\boldsymbol{U}_\mathcal{G} \otimes \boldsymbol{U}_\mathcal{H})\, \boldsymbol{\Lambda}_{\mathcal{G}\circ\mathcal{H}}\, (\boldsymbol{U}_\mathcal{G} \otimes \boldsymbol{U}_\mathcal{H})^\top \\
&= (\boldsymbol{U}_\mathcal{G} \otimes \boldsymbol{U}_\mathcal{H})\, (\boldsymbol{\Lambda}_\mathcal{G} \otimes \boldsymbol{\Lambda}_\mathcal{H})\, (\boldsymbol{U}_\mathcal{G} \otimes \boldsymbol{U}_\mathcal{H})^\top \\
&= ((\boldsymbol{U}_\mathcal{G}\boldsymbol{\Lambda}_\mathcal{G}) \otimes (\boldsymbol{U}_\mathcal{H}\boldsymbol{\Lambda}_\mathcal{H}))\left(\boldsymbol{U}_\mathcal{G}^\top \otimes \boldsymbol{U}_\mathcal{H}^\top\right) \\
&= \left(\boldsymbol{U}_\mathcal{G}\boldsymbol{\Lambda}_\mathcal{G}\boldsymbol{U}_\mathcal{G}^\top\right) \otimes \left(\boldsymbol{U}_\mathcal{H}\boldsymbol{\Lambda}_\mathcal{H}\boldsymbol{U}_\mathcal{H}^\top\right) \\
&= \boldsymbol{G} \otimes \boldsymbol{H}
\end{aligned} \tag{2}$$

B.2. Cartesian Graph Product

Now suppose $x \circ y = x + y$, it is not hard to see $\boldsymbol{\Lambda}_{\mathcal{G}\circ\mathcal{H}} = \boldsymbol{\Lambda}_\mathcal{G} \otimes \boldsymbol{I}_n + \boldsymbol{I}_m \otimes \boldsymbol{\Lambda}_\mathcal{H}$. By similar analysis as above we have $\boldsymbol{G} \circ \boldsymbol{H} = \boldsymbol{G} \otimes \boldsymbol{I}_n + \boldsymbol{I}_m \otimes \boldsymbol{H} = \boldsymbol{G} \oplus \boldsymbol{H}$.

C. Proof of Proposition 1

Optimization (7) is equivalent to (1) when $\circ$ is the Cartesian graph product, $C_0 = C_1 + 2C_2$ and $\kappa(z) = \left(1 - \frac{C_2}{C_0} z\right)^{-1}$.

[1] The "vec" operator concatenates the rows of a matrix into a single vector.

Proof. In this case, $\kappa(\boldsymbol{G} \circ \boldsymbol{H}) = \left(\boldsymbol{I} - \frac{C_2}{C_0}(\boldsymbol{G} \oplus \boldsymbol{H})\right)^{-1}$.

We assume that both $\boldsymbol{G}$ and $\boldsymbol{H}$ have been symmetrically normalized during preprocessing, i.e. $\mathcal{L}_{\mathcal{G}} = \boldsymbol{I} - \boldsymbol{G}$ and $\mathcal{L}_{\mathcal{H}} = \boldsymbol{I} - \boldsymbol{H}$. Consider the regularization term in (1)

$$
\begin{aligned}
&\frac{C_0}{2}\mathrm{vec}(\boldsymbol{F})^\top [\kappa(\boldsymbol{G} \circ \boldsymbol{H})]^{-1} \mathrm{vec}(\boldsymbol{F}) \\
=&\frac{C_0}{2}\mathrm{vec}(\boldsymbol{F})^\top \left(\boldsymbol{I} - \frac{C_2}{C_0}(\boldsymbol{G} \oplus \boldsymbol{H})\right) \mathrm{vec}(\boldsymbol{F}) \\
=&\frac{C_0}{2}\|\boldsymbol{F}\|_{\mathrm{F}}^2 - \frac{C_2}{2}\mathrm{vec}(\boldsymbol{F})^\top (\boldsymbol{G} \oplus \boldsymbol{H}) \mathrm{vec}(\boldsymbol{F}) \\
=&\frac{C_0}{2}\|\boldsymbol{F}\|_{\mathrm{F}}^2 - \frac{C_2}{2}\mathrm{vec}(\boldsymbol{F})^\top (\boldsymbol{G} \otimes \boldsymbol{I}_n + \boldsymbol{I}_m \otimes \boldsymbol{H}) \mathrm{vec}(\boldsymbol{F}) \\
=&\frac{C_0}{2}\|\boldsymbol{F}\|_{\mathrm{F}}^2 - \frac{C_2}{2}\left[\mathrm{tr}\left(\boldsymbol{F}^\top \boldsymbol{G}\boldsymbol{F}\right) + \mathrm{tr}\left(\boldsymbol{F}\boldsymbol{H}\boldsymbol{F}^\top\right)\right] \\
=&\frac{C_1}{2}\|\boldsymbol{F}\|_{\mathrm{F}}^2 + \frac{C_2}{2}\left[2\|\boldsymbol{F}\|_{\mathrm{F}}^2 - \mathrm{tr}\left(\boldsymbol{F}^\top \boldsymbol{G}\boldsymbol{F}\right) - \mathrm{tr}\left(\boldsymbol{F}\boldsymbol{H}\boldsymbol{F}^\top\right)\right] \\
=&\frac{C_1}{2}\|\boldsymbol{F}\|_{\mathrm{F}}^2 + \frac{C_2}{2}\left[\mathrm{tr}\left(\boldsymbol{F}^\top (\boldsymbol{I} - \boldsymbol{G})\boldsymbol{F}\right) + \mathrm{tr}\left(\boldsymbol{F}(\boldsymbol{I} - \boldsymbol{H})\boldsymbol{F}^\top\right)\right] \\
=&\frac{C_1}{2}\|\boldsymbol{F}\|_{\mathrm{F}}^2 + \frac{C_2}{2}\mathrm{tr}\left(\boldsymbol{F}^\top \mathcal{L}_{\mathcal{G}}\boldsymbol{F}\right) + \frac{C_2}{2}\mathrm{tr}\left(\boldsymbol{F}\mathcal{L}_{\mathcal{H}}\boldsymbol{F}^\top\right)
\end{aligned}
$$

Plugging back the above expression to optimization (1) closes the proof. □

D. Proof of Lemma 1

If $\circ$ defines a spectral graph product (SGP), then

$$
\varphi_{\circ,\kappa}(\boldsymbol{F}) := \mathrm{vec}^{-1}\left([\kappa(\boldsymbol{G} \circ \boldsymbol{H})]^{-1}\mathrm{vec}(\boldsymbol{F})\right) = \boldsymbol{U}_{\mathcal{G}}\left[\boldsymbol{\Sigma}_{\circ,\kappa} * \left(\boldsymbol{U}_{\mathcal{G}}^\top \boldsymbol{F}\boldsymbol{U}_{\mathcal{H}}\right)\right]\boldsymbol{U}_{\mathcal{H}}^\top \tag{3}
$$

where $*$ is the matrix Hadamard (a.k.a. element-wise) product, $\boldsymbol{\Sigma}_{\circ,\kappa}$ is a $m \times n$ matrix with each element defined as

$$
[\boldsymbol{\Sigma}_{\circ,\kappa}]_{ij} = 1 \Big/ \kappa\left([\lambda_{\mathcal{G}}]_i \circ [\lambda_{\mathcal{H}}]_j\right) \tag{4}
$$

Proof. First, let us derive the eigendecomposition of $[\kappa(\boldsymbol{G} \circ \boldsymbol{H})]^{-1}$.

According to Definition 5, $\boldsymbol{G} \circ \boldsymbol{H}$ has the eigendecomposition $(\boldsymbol{U}_{\mathcal{G}} \otimes \boldsymbol{U}_{\mathcal{H}})\boldsymbol{\Lambda}_{\mathcal{G}\circ\mathcal{H}}(\boldsymbol{U}_{\mathcal{G}} \otimes \boldsymbol{U}_{\mathcal{H}})^\top$ where $[\boldsymbol{\Lambda}_{\mathcal{G}\circ\mathcal{H}}]_{(i,j),(i,j)} = [\lambda_{\mathcal{G}}]_i \circ [\lambda_{\mathcal{H}}]_j$. Since κ is a spectral transformation, we can directly apply it to the eigenvalues of $\boldsymbol{G} \circ \boldsymbol{H}$. Therefore

$$
\begin{aligned}
[\kappa(\boldsymbol{G} \circ \boldsymbol{H})]^{-1} &= \left[\kappa\left((\boldsymbol{U}_{\mathcal{G}} \otimes \boldsymbol{U}_{\mathcal{H}})\boldsymbol{\Lambda}_{\mathcal{G}\circ\mathcal{H}}(\boldsymbol{U}_{\mathcal{G}} \otimes \boldsymbol{U}_{\mathcal{H}})^\top\right)\right]^{-1} \\
&= \left[(\boldsymbol{U}_{\mathcal{G}} \otimes \boldsymbol{U}_{\mathcal{H}})\kappa(\boldsymbol{\Lambda}_{\mathcal{G}\circ\mathcal{H}})(\boldsymbol{U}_{\mathcal{G}} \otimes \boldsymbol{U}_{\mathcal{H}})^\top\right]^{-1} \\
&= (\boldsymbol{U}_{\mathcal{G}} \otimes \boldsymbol{U}_{\mathcal{H}})[\kappa(\boldsymbol{\Lambda}_{\mathcal{G}\circ\mathcal{H}})]^{-1}\left(\boldsymbol{U}_{\mathcal{G}}^\top \otimes \boldsymbol{U}_{\mathcal{H}}^\top\right) \\
&= (\boldsymbol{U}_{\mathcal{G}} \otimes \boldsymbol{U}_{\mathcal{H}})\,\mathrm{diag}(\mathrm{vec}(\boldsymbol{\Sigma}_{\circ,\kappa}))\left(\boldsymbol{U}_{\mathcal{G}}^\top \otimes \boldsymbol{U}_{\mathcal{H}}^\top\right)
\end{aligned} \tag{5}
$$

The last equality follows the definition of $\boldsymbol{\Sigma}_{\circ,\kappa}$ in (4).

Now, let us derive the expression for $\mathrm{vec}\left(\varphi_{\circ,\kappa}\left(\boldsymbol{F}\right)\right)$

$$\begin{aligned}
\mathrm{vec}\left(\varphi_{\circ,\kappa}\left(\boldsymbol{F}\right)\right) &= \left[\kappa\left(\boldsymbol{G}\circ\boldsymbol{H}\right)\right]^{-1}\mathrm{vec}\left(\boldsymbol{F}\right)\\
&= \left(\boldsymbol{U}_{\mathcal{G}}\otimes\boldsymbol{U}_{\mathcal{H}}\right)\mathrm{diag}\left(\mathrm{vec}\left(\boldsymbol{\Sigma}_{\circ,\kappa}\right)\right)\left(\boldsymbol{U}_{\mathcal{G}}^{\top}\otimes\boldsymbol{U}_{\mathcal{H}}^{\top}\right)\mathrm{vec}\left(\boldsymbol{F}\right)\\
&= \left(\boldsymbol{U}_{\mathcal{G}}\otimes\boldsymbol{U}_{\mathcal{H}}\right)\mathrm{diag}\left(\mathrm{vec}\left(\boldsymbol{\Sigma}_{\circ,\kappa}\right)\right)\mathrm{vec}\left(\boldsymbol{U}_{\mathcal{G}}^{\top}\boldsymbol{F}\boldsymbol{U}_{\mathcal{H}}\right)\\
&= \left(\boldsymbol{U}_{\mathcal{G}}\otimes\boldsymbol{U}_{\mathcal{H}}\right)\mathrm{vec}\left[\boldsymbol{\Sigma}_{\circ,\kappa}*\left(\boldsymbol{U}_{\mathcal{G}}^{\top}\boldsymbol{F}\boldsymbol{U}_{\mathcal{H}}\right)\right]\\
&= \mathrm{vec}\left(\boldsymbol{U}_{\mathcal{G}}\left[\boldsymbol{\Sigma}_{\circ,\kappa}*\left(\boldsymbol{U}_{\mathcal{G}}^{\top}\boldsymbol{F}\boldsymbol{U}_{\mathcal{H}}\right)\right]\boldsymbol{U}_{\mathcal{H}}^{\top}\right)
\end{aligned} \tag{6}$$

The lemma follows by applying vec^{-1} to both sides of the equation above. □

E. Proof of Theorem 1

For brevity we write $\boldsymbol{\Sigma}_{\circ,\kappa}$ as $\boldsymbol{\Sigma}$.

Suppose $\circ$ is a spectral graph product. Let $\sum_{k}^{\mathrm{rank}(\boldsymbol{\Sigma})} c_k\boldsymbol{u}_k\boldsymbol{v}_k^{\top}$ be the eigendecomposition of $\boldsymbol{\Sigma}$, and $r\left(\boldsymbol{G},\boldsymbol{u}\right)$ be matrix $\boldsymbol{G}$ with its eigenvalues replaced by some other vector $\boldsymbol{u}$. We have

$$\varphi_{\circ,\kappa}\left(\boldsymbol{F}\right) = \sum_{k=1}^{\mathrm{rank}(\boldsymbol{\Sigma})} c_k r\left(\boldsymbol{G},\boldsymbol{u}_k\right)\boldsymbol{F}r\left(\boldsymbol{H},\boldsymbol{v}_k\right) \tag{7}$$

Proof. From Lemma 1 we have

$$\begin{aligned}
\varphi_{\circ,\kappa}\left(\boldsymbol{F}\right) &= \boldsymbol{U}_{\mathcal{G}}\left[\boldsymbol{\Sigma}*\left(\boldsymbol{U}_{\mathcal{G}}^{\top}\boldsymbol{F}\boldsymbol{U}_{\mathcal{H}}\right)\right]\boldsymbol{U}_{\mathcal{H}}^{\top}\\
&= \boldsymbol{U}_{\mathcal{G}}\left[\left(\sum_{k=1}^{\mathrm{rank}(\boldsymbol{\Sigma})} c_k\boldsymbol{u}_k\boldsymbol{v}_k^{\top}\right)*\left(\boldsymbol{U}_{\mathcal{G}}^{\top}\boldsymbol{F}\boldsymbol{U}_{\mathcal{H}}\right)\right]\boldsymbol{U}_{\mathcal{H}}^{\top}\\
&= \sum_{k=1}^{\mathrm{rank}(\boldsymbol{\Sigma})} c_k\boldsymbol{U}_{\mathcal{G}}\left[\left(\boldsymbol{u}_k\boldsymbol{v}_k^{\top}\right)*\left(\boldsymbol{U}_{\mathcal{G}}^{\top}\boldsymbol{F}\boldsymbol{U}_{\mathcal{H}}\right)\right]\boldsymbol{U}_{\mathcal{H}}^{\top}\\
&= \sum_{k=1}^{\mathrm{rank}(\boldsymbol{\Sigma})} c_k\boldsymbol{U}_{\mathcal{G}}\left[\mathrm{diag}\left(\boldsymbol{u}_k\right)\left(\boldsymbol{U}_{\mathcal{G}}^{\top}\boldsymbol{F}\boldsymbol{U}_{\mathcal{H}}\right)\mathrm{diag}\left(\boldsymbol{v}_k\right)\right]\boldsymbol{U}_{\mathcal{H}}^{\top}\\
&= \sum_{k=1}^{\mathrm{rank}(\boldsymbol{\Sigma})} c_k\left(\boldsymbol{U}_{\mathcal{G}}\mathrm{diag}\left(\boldsymbol{u}_k\right)\boldsymbol{U}_{\mathcal{G}}^{\top}\right)\boldsymbol{F}\left(\boldsymbol{U}_{\mathcal{H}}\mathrm{diag}\left(\boldsymbol{v}_k\right)\boldsymbol{U}_{\mathcal{H}}^{\top}\right)\\
&= \sum_{k=1}^{\mathrm{rank}(\boldsymbol{\Sigma})} c_k r\left(\boldsymbol{G},\boldsymbol{u}_k\right)\boldsymbol{F}r\left(\boldsymbol{H},\boldsymbol{v}_k\right)
\end{aligned} \tag{8}$$

□

F. Proof of Corollary 1

If there exists σ_1,σ_2 such that for all $x,y\in\mathbb{R}$, $\frac{1}{\kappa(x\circ y)}\equiv\sigma_1\left(x\right)\sigma_2\left(y\right)$. Then

$$\varphi_{\circ,\kappa}\left(\boldsymbol{F}\right) = \sigma_1\left(\boldsymbol{G}\right)\boldsymbol{F}\sigma_2\left(\boldsymbol{H}\right) \tag{9}$$

If there exits σ_1, σ_2 such that for all $x,y\in\mathbb{R}$, $\frac{1}{\kappa(x\circ y)}\equiv\sigma_1\left(x\right)+\sigma_2\left(y\right)$. Then

$$\varphi_{\circ,\kappa}\left(\boldsymbol{F}\right) = \sigma_1\left(\boldsymbol{G}\right)\boldsymbol{F}+\boldsymbol{F}\sigma_2\left(\boldsymbol{H}\right) \tag{10}$$

Proof. Define $\sigma_1(\boldsymbol{\lambda}) := (\sigma_1(\lambda_1), \ldots \sigma_1(\lambda_m))$ and $\sigma_2(\boldsymbol{\mu}) := (\sigma_2(\mu_1), \ldots \sigma_2(\mu_n))$. Notice

- $r(\boldsymbol{G}, \mathbf{1}) \equiv \mathbf{1}$.
- $r(\boldsymbol{G}, \sigma(\boldsymbol{u})) \equiv \sigma(\boldsymbol{G})$ if $\boldsymbol{u}$ is the eigenvalues of $\boldsymbol{G}$.

The first condition $\frac{1}{\kappa(x \circ y)} \equiv \sigma_1(x)\sigma_2(y)$ implies that $\boldsymbol{\Sigma} = 1 \cdot \sigma_1(\boldsymbol{\lambda})\sigma_2(\boldsymbol{\mu})^\top$, and the conclusion follows Theorem 1 with $\mathrm{rank}(\boldsymbol{\Sigma}) = 1$, $c_1 = 1$, $\boldsymbol{u}_1 = \sigma_1(\boldsymbol{\lambda})$ and $\boldsymbol{v}_1 = \sigma_2(\boldsymbol{\mu})$.

The second condition $\frac{1}{\kappa(x \circ y)} \equiv \sigma_1(x) + \sigma_2(y)$ implies that $\boldsymbol{\Sigma} = 1 \cdot \sigma_1(\boldsymbol{\lambda})\mathbf{1}_n^\top + 1 \cdot \mathbf{1}_m \sigma_2(\boldsymbol{\mu})^\top$. The conclusion follows Theorem 1 with $\mathrm{rank}(\boldsymbol{\Sigma}) = 2$, $c_1 = c_2 = 1$, $\boldsymbol{u}_1 = \sigma_1(\boldsymbol{\lambda})$, $\boldsymbol{v}_1 = \mathbf{1}_n$, $\boldsymbol{u}_2 = \mathbf{1}_m$ and $\boldsymbol{v}_2 = \sigma_2(\boldsymbol{\mu})$. $\square$