Supplementary Material for "Graph Coarsening with Preserved Spectral Properties"

A Proof of Property 4.2, 4.3

Proof. We start by noticing that the projection matrix $\mathbf{\Pi}$ acts as an identity matrix w.r.t. the lifted normalized Laplacian $\boldsymbol{\mathcal{L}}_l = \mathbf{\Pi}\boldsymbol{\mathcal{L}}_l\mathbf{\Pi}$, since $\boldsymbol{\mathcal{L}}_l = \boldsymbol{C}^\top \boldsymbol{\mathcal{L}}_c \boldsymbol{C} = \boldsymbol{C}^\top \boldsymbol{C} \boldsymbol{\mathcal{L}}_l \boldsymbol{C}^\top \boldsymbol{C} = \mathbf{\Pi}\boldsymbol{\mathcal{L}}_l\mathbf{\Pi}$. Now, consider the following eigenvalue equation:

$$
\begin{aligned}
\boldsymbol{\mathcal{L}}_c \boldsymbol{u}_c &= \lambda_c \boldsymbol{u}_c \\
\boldsymbol{C}\boldsymbol{\mathcal{L}}_l \boldsymbol{C}^\top \boldsymbol{u}_c &= \lambda_c \boldsymbol{u}_c \\
\boldsymbol{C}^\top \boldsymbol{C}\boldsymbol{\mathcal{L}}_l \boldsymbol{C}^\top \boldsymbol{u}_c &= \lambda_c \boldsymbol{C}^\top \boldsymbol{u}_c \\
\mathbf{\Pi}\boldsymbol{\mathcal{L}}_l \mathbf{\Pi}\boldsymbol{C}^\top \boldsymbol{u}_c &= \lambda_c \boldsymbol{C}^\top \boldsymbol{u}_c \\
\boldsymbol{\mathcal{L}}_l \boldsymbol{C}^\top \boldsymbol{u}_c &= \lambda_c \boldsymbol{C}^\top \boldsymbol{u}_c
\end{aligned}
$$

Note that in the fourth step, we used the relation $\boldsymbol{C}^\top = \boldsymbol{C}^\top \boldsymbol{C} \boldsymbol{C}^\top = \mathbf{\Pi}\boldsymbol{C}^\top$, which holds due to the properties of the Moore-Penrose pseudo-inverse. Thus, $\boldsymbol{C}^\top \boldsymbol{u}_c$ are eigenvectors of $\boldsymbol{\mathcal{L}}_l$ with the corresponding eigenvalues of the coarse graph.

To show there are $N-n$ additional eigenvalues 1, one can observe that $\boldsymbol{I}_N - \boldsymbol{\mathcal{L}} = \boldsymbol{D}_l^{-1/2}\boldsymbol{W}_l\boldsymbol{D}_l^{-1/2}$ is a rank-n matrix because nodes within the same partition have exactly the same edge weights. Hence $\boldsymbol{I}_N - \boldsymbol{\mathcal{L}}$ contains $N-1$ eigenvalue 0 and correspondingly $\boldsymbol{\mathcal{L}}$ contains eigenvalue 1 with $N-n$ multiplicity. ☐

B Proof of Proposition 4.1, 4.2

For the simplicity of the proof, we use the $\boldsymbol{\mathcal{L}}^{rw} = \boldsymbol{I} - \boldsymbol{D}^{-1}\boldsymbol{W}$ to replace the original normalized Laplacian $\boldsymbol{\mathcal{L}}$ to compute the Laplacian eigenvalues. Note that $\boldsymbol{\mathcal{L}}^{rw}$ has the same set of eigenvalues as the original normalized Laplacian $\boldsymbol{\mathcal{L}}$ and the relation of the eigenvalues and eigenvectors satisfy,

$$
\boldsymbol{\mathcal{L}}^{rw} = \boldsymbol{D}^{-1/2}\boldsymbol{\mathcal{L}}\boldsymbol{D}^{1/2}, \quad \boldsymbol{u}^{rw} = \boldsymbol{D}^{-1/2}\boldsymbol{u}
$$

B.1 Proof of Proposition 4.1

Proof. We show that under the assumption above, the eigenvalues of the original normalized Laplacian contain the eigenvalues of coarse graph $\mathcal{G}_c$ plus eigenvalue 1 with $N-n$ multiplicities.

The random-walk Laplacian of the coarse graph satisfies,

$$
\begin{aligned}
\boldsymbol{\mathcal{L}}_c^{rw} &= \boldsymbol{I}_n - \boldsymbol{D}_c^{-1}\boldsymbol{W}_c \\
&= \boldsymbol{P}\boldsymbol{I}_N\boldsymbol{P}^{\mp} - \boldsymbol{P}\boldsymbol{D}\boldsymbol{P}^{\mp}\boldsymbol{P}\boldsymbol{W}\boldsymbol{P}^{\mp} \\
&= \boldsymbol{P}\boldsymbol{I}_N\boldsymbol{P}^{\mp} - \boldsymbol{P}\boldsymbol{D}^{-1}\boldsymbol{W}\boldsymbol{P}^{\mp} \\
&= \boldsymbol{P}(\boldsymbol{I}_N - \boldsymbol{D}^{-1}\boldsymbol{W})\boldsymbol{P}^{\mp} \\
&= \boldsymbol{P}\boldsymbol{\mathcal{L}}^{rw}\boldsymbol{P}^{\mp}
\end{aligned}
$$

The third equation holds because of the assumption in Equation (9). Then, the eigenvalue and eigenvector of $\boldsymbol{\mathcal{L}}_c^{rw}$ satisfy the following:

$$
\begin{aligned}
\boldsymbol{\mathcal{L}}_c^{rw}\boldsymbol{u}^{rw} &= \lambda \boldsymbol{u}_c^{rw} \\
\boldsymbol{P}\boldsymbol{\mathcal{L}}^{rw}\boldsymbol{P}^{\mp}\boldsymbol{u}^{rw} &= \lambda \boldsymbol{u}_c^{rw} \\
\boldsymbol{P}^{\mp}\boldsymbol{P}\boldsymbol{\mathcal{L}}^{rw}\boldsymbol{P}^{\mp}\boldsymbol{u}^{rw} &= \lambda \boldsymbol{P}^{\mp}\boldsymbol{u}_c^{rw} \\
\boldsymbol{\mathcal{L}}^{rw}\boldsymbol{P}^{\mp}\boldsymbol{u}^{rw} &= \lambda \boldsymbol{P}^{\mp}\boldsymbol{u}_c^{rw}
\end{aligned}
$$

that is, $\boldsymbol{\mathcal{L}}^{rw}$ has the eigenvalue λ with the corresponding eigenvector $\boldsymbol{P}^{\mp}\boldsymbol{u}^{rw}$.

To see that the original graph contains $N-n$ eigenvalue 1, we consider $\boldsymbol{D}^{-1}\boldsymbol{W} = \boldsymbol{I}_N - \boldsymbol{\mathcal{L}}^{rw}$ which consists of rows of normalized edge weights with row i as $\frac{\boldsymbol{w}(i)}{d(i)}$. From the assumption in Equation (9), we have identical rows for each partition $\mathcal{S}_r$. Thus $\boldsymbol{D}^{-1}\boldsymbol{W}$ is at most rank-n, which indicates $\boldsymbol{\mathcal{L}}^{rw}$ contains $N-n$ eigenvalue 1.

Thus, the original normalized Laplacian has the same eigenvalues as the lifted graph. Both definition of spectral distances are 0. □

B.2 Proof of Proposition 4.2

Proof. The normalized Laplacian of the original graph can be viewed as a perturbation of the normalized Laplacian of the lifted graph as

$$\boldsymbol{\mathcal{L}}^{rw} = \boldsymbol{\mathcal{L}}_l^{rw} + \boldsymbol{E},$$

where $\boldsymbol{E}$ is the perturbation matrix.

We expand the entries of $\boldsymbol{\mathcal{L}}^{rw}$ as follows:

$$\boldsymbol{\mathcal{L}}^{rw}(i,j) = \boldsymbol{I}(i,j) - \frac{\boldsymbol{W}(i,j)}{d(i)}.$$

As the coarse graph is coarsened from merging one pair of nodes, the edge weights of the lifted graph $\mathcal{G}_l$ can be expressed as,

$$\boldsymbol{W}_l(i,j) = \begin{cases} \frac{\boldsymbol{W}(a,a)+\boldsymbol{W}(a,b)+\boldsymbol{W}(b,a)+\boldsymbol{W}(b,b)}{4} & \text{if } i \in \{a,b\} \text{ and } j \in \{a,b\} \\ \frac{\boldsymbol{W}(a,j)+\boldsymbol{W}(b,j)}{2} & \text{if } i \in \{a,b\} \text{ and } j \notin \{a,b\} \\ \frac{\boldsymbol{W}(i,a)+\boldsymbol{W}(i,b)}{2} & \text{if } i \notin \{a,b\} \text{ and } j \in \{a,b\} \\ \boldsymbol{W}(i,j) & \text{otherwise.} \end{cases}$$

and the corresponding node degree d_l is

$$d_l(i) = \begin{cases} \frac{d(a)+d(b)}{2} & \text{if } i \in \{a,b\} \\ d(i) & \text{otherwise.} \end{cases}$$

The above imply that $\boldsymbol{\mathcal{L}}_l^{rw}$ can be expanded as follows:

$$\boldsymbol{\mathcal{L}}_l^{rw} = \boldsymbol{I}(i,j) - \frac{\boldsymbol{W}_l(i,j)}{d_l(i)} = \begin{cases} \boldsymbol{I}(i,j) - \frac{\boldsymbol{W}(a,a)+\boldsymbol{W}(a,b)+\boldsymbol{W}(b,a)+\boldsymbol{W}(b,b)}{2(d(a)+d(b))} & \text{if } i \in \{a,b\} \text{ and } j \in \{a,b\} \\ \boldsymbol{I}(i,j) - \frac{\boldsymbol{W}(a,j)+\boldsymbol{W}(b,j)}{d(a)+d(b)} & \text{if } i \in \{a,b\} \text{ and } j \notin \{a,b\} \\ \boldsymbol{I}(i,j) - \frac{\boldsymbol{W}(i,a)+\boldsymbol{W}(i,b)}{2d(i)} & \text{if } i \notin \{a,b\} \text{ and } j \in \{a,b\} \\ \boldsymbol{I}(i,j) - \frac{\boldsymbol{W}(i,j)}{d(i)} & \text{otherwise} \end{cases}$$

and the perturbation matrix $\boldsymbol{E} = \boldsymbol{\mathcal{L}}^{rw} - \boldsymbol{\mathcal{L}}_l^{rw}$ is given by

$$\boldsymbol{E}(i,j) = \begin{cases} \frac{\boldsymbol{W}(i,j)}{d(i)} - \frac{\boldsymbol{W}(a,a)+\boldsymbol{W}(a,b)+\boldsymbol{W}(b,a)+\boldsymbol{W}(b,b)}{2(d(a)+d(b))} & \text{if } i \in \{a,b\} \text{ and } j \in \{a,b\} \\ \frac{\boldsymbol{W}(i,j)}{d(i)} - \frac{\boldsymbol{W}(a,j)+\boldsymbol{W}(b,j)}{d(a)+d(b)} & \text{if } i \in \{a,b\} \text{ and } j \notin \{a,b\} \\ \frac{\boldsymbol{W}(i,j)}{d(i)} - \frac{\boldsymbol{W}(i,a)+\boldsymbol{W}(i,b)}{2d(i)} & \text{if } i \notin \{a,b\} \text{ and } j \in \{a,b\} \\ 0 & \text{otherwise.} \end{cases}$$

From Weyl (1912), we have the following bound on the eigenvalue gap between $\boldsymbol{\lambda}(i)$ and $\boldsymbol{\lambda}_l(i)$:

$$|\boldsymbol{\lambda}(i) - \boldsymbol{\lambda}_l(i)| \leq \|E\|_2$$

Moreover, Wolkowicz and Styan (1980) proved that the spectral norm $\|E\|_2$ admits the simple upper bound:

$$\|\boldsymbol{E}\|_2^2 \leq \max_{i,j} \boldsymbol{r}_i \boldsymbol{c}_j = \max_i \boldsymbol{r}_i \max_j \boldsymbol{c}_j,$$

where $\boldsymbol{r}_i = \sum_j |\boldsymbol{E}(i,j)|$ and $\boldsymbol{c}_j = \sum_i |\boldsymbol{E}(i,j)|$.

Let us focus on term $\boldsymbol{r}_i$.

Case 1: $i \notin \{a, b\}$,

$$\begin{aligned}\boldsymbol{r}_i &= |\frac{\boldsymbol{W}(i,a)}{d(i)} - \frac{\boldsymbol{W}(i,a)+\boldsymbol{W}(i,b)}{2d(i)}| + |\frac{\boldsymbol{W}(i,a)}{d(i)} - \frac{\boldsymbol{W}(i,a)+\boldsymbol{W}(i,b)}{2d(i)}| \\ &= |\frac{\boldsymbol{W}(i,a)}{d(i)} - \frac{\boldsymbol{W}(i,b)}{d(i)}| \leq \left\| \frac{\boldsymbol{W}(i,a)}{d(i)} - \frac{\boldsymbol{W}(i,b)}{d(i)} \right\|_1 \leq \epsilon\end{aligned}$$

Case 2: $i \in \{a, b\}$, and suppose $d(a) \leq d(b)$ w.l.o.g.,

$$\begin{aligned}\boldsymbol{r}_i &= |\frac{\boldsymbol{W}(i,a)}{d(i)} - \frac{\boldsymbol{W}(a,a)+\boldsymbol{W}(a,b)+\boldsymbol{W}(b,a)+\boldsymbol{W}(b,b)}{2(d(a)+d(b))}| + |\frac{\boldsymbol{W}(i,b)}{d(i)} - \frac{\boldsymbol{W}(a,a)+\boldsymbol{W}(a,b)+\boldsymbol{W}(b,a)+\boldsymbol{W}(b,b)}{2(d(a)+d(b))}| \\ &+ \sum_{j \notin \{a,b\}} |\frac{\boldsymbol{W}(i,j)}{d(i)} - \frac{\boldsymbol{W}(a,j)+\boldsymbol{W}(b,j)}{d(a)+d(b)}| \\ &\leq |\frac{\boldsymbol{W}(a,a)}{d(a)} - \frac{\boldsymbol{W}(b,a)}{d(b)}| + |\frac{\boldsymbol{W}(a,b)}{d(a)} - \frac{\boldsymbol{W}(b,b)}{d(b)}| + \sum_{j \notin \{a,b\}} |\frac{\boldsymbol{W}(a,j)}{d(a)} - \frac{\boldsymbol{W}(b,j)}{d(b)}| \\ &= \left\| \frac{\boldsymbol{W}(i,a)}{d(i)} - \frac{\boldsymbol{W}(i,b)}{d(i)} \right\|_1 \leq \epsilon \qquad (1)\end{aligned}$$

We have $\max_i \boldsymbol{r}_i \leq \epsilon$. Similarly, we can show that $\boldsymbol{c}_j \leq \epsilon$. The spectral norm of the perturbation matrix $\boldsymbol{E}$ then is bounded by

$$\|\boldsymbol{E}\|_2 \leq \sqrt{\max_i \boldsymbol{r}_i \max_j \boldsymbol{c}_j} \leq \epsilon. \qquad (2)$$

Combining the above, we have the bound of each term in the spectral distance as,

$$|\boldsymbol{\lambda}(i) - \boldsymbol{\lambda}_l(i)| \leq \epsilon \qquad (3)$$

The bounds of the full and partial spectral distance follow the Equation 3 as they contain N and n eigengap terms respectively. □

C Proof of Corollary 5.1

Proof. We denote the intermediate graphs at iteration s as $\mathcal{G}^{(s)}$ with $\mathcal{G}^{(N)}$ as the original graph $\mathcal{G}$ and $\mathcal{G}^{(n)}$ as the coarse graph $\mathcal{G}_c$. From Proposition 4.2 and the spectral distance is a distance metric over the Laplacian eigenvalues, we have the following,

$$SD_{full}(\mathcal{G}, \mathcal{G}_c) \leq \sum_{s=N}^{n+1} SD_{full}(\mathcal{G}^{(s)}, \mathcal{G}^{(s-1)}) \leq N \sum_{s=N}^{n+1} \epsilon_s$$

and

$$SD_{part}(\mathcal{G}, \mathcal{G}_c) \leq \sum_{s=N}^{n+1} SD_{part}(\mathcal{G}^{(s)}, \mathcal{G}^{(s-1)}) \leq N \sum_{s=N}^{n+1} \epsilon_s$$

□

D Proof of Theorem 5.2

Proof. We rewrite the objective of the k-means algorithm as the following,

$$\mathcal{F}(\boldsymbol{U}, \mathcal{P}) = \sum_{i=1}^{N} \left(\boldsymbol{r}(i) - \sum_{j \in \mathcal{S}_i} \frac{\boldsymbol{r}(j)}{|\mathcal{S}_i|} \right)^2 = \|\boldsymbol{U} - \boldsymbol{C}\boldsymbol{C}^\top \boldsymbol{U}\|_F^2,$$

where the matrix $\boldsymbol{C} \in \mathbb{R}^{n\times N}$ is the normalized coarsening matrix corresponding to the graph partition $\mathcal{P}$. With the notation $\boldsymbol{\Pi} = \boldsymbol{C}\boldsymbol{C}^\top$ and $\boldsymbol{\Pi}^\perp = \boldsymbol{I} - \boldsymbol{\Pi}$ from Section 3.2, the k-means objective is written as

$$\mathcal{F}(\boldsymbol{U}, \mathcal{P}) = \|\boldsymbol{\Pi}^\perp \boldsymbol{U}\|_F^2.$$

We express the partial spectral distance as in Definition 4.5

$$SD_{\text{part}}(\mathcal{G}, \mathcal{G}_c) = \sum_{i=1}^{k_1}(\boldsymbol{\lambda}_c(i) - \boldsymbol{\lambda}(i)) + \sum_{j=k_2+1}^{N}(\boldsymbol{\lambda}(j) - \boldsymbol{\lambda}_c(j+n-N)) \tag{4}$$

where $k_1 = \arg\max_i\{i : \boldsymbol{\lambda}_c(i) < 1\}, k_2 = N - n + k_1$.

Because of the interlacing property 4.1, we remove the absolute sign on the terms.

Correspondingly, we separate the k-means cost in two terms as,

$$\mathcal{F}(\boldsymbol{U}, \boldsymbol{C}) = \|\boldsymbol{U}_{k_1} - \boldsymbol{C}\boldsymbol{C}^\top \boldsymbol{U}_{k_1}\|_F^2 + \|\boldsymbol{U}'_{k_2} - \boldsymbol{C}\boldsymbol{C}^\top \boldsymbol{U}'_{k_2}\|_F^2 = \|\boldsymbol{\Pi}^\perp \boldsymbol{U}_{k_1}\|_F^2 + \|\boldsymbol{\Pi}^\perp \boldsymbol{U}'_{k_2}\|_F^2$$

where $\boldsymbol{U}_{k_1}$ and $\boldsymbol{U}'_{k_2}$ denote the eigenvectors corresponding to the smallest k_1 and largest $n - k_1$ eigenvalues of the original graph. We also denote $\delta_{k_1} = \|\boldsymbol{\Pi}^\perp \boldsymbol{U}_{k_1}\|_F^2$ and $\delta'_{k_2} = \|\boldsymbol{\Pi}^\perp \boldsymbol{U}'_{k_2}\|_F^2$.

We will prove the results of the two terms separately.

For the first k_1 eigenvalue gaps, we start by the following generalization of the Courant-Fisher theorem:

$$\sum_{i\le k_1} \boldsymbol{\lambda}_c(i) = \min_{\boldsymbol{V}^\top \boldsymbol{V} = \boldsymbol{I}_k} \operatorname{tr}(\boldsymbol{V}^\top \boldsymbol{\mathcal{L}}_c \boldsymbol{V}).$$

We write $\boldsymbol{\mathcal{L}} = \boldsymbol{S}^\top \boldsymbol{S}$ where $\boldsymbol{S} \in \mathbb{R}^{M\times N}$ denotes the incidence matrix of the normalized Laplacian $\boldsymbol{\mathcal{L}}$ with the following form

$$\boldsymbol{S}(v, e) = \begin{cases} \frac{1}{\sqrt{d(i)}}, \text{if } v = i \\ -\frac{1}{\sqrt{d(j)}}, \text{if } v = j, \end{cases}$$

where $e \in \mathcal{E}$ with i and j as the connecting nodes. Then, the first k_1 eigenvalues are

$$\sum_{i\le k_1} \boldsymbol{\lambda}_c(i) = \min_{\boldsymbol{V}^\top \boldsymbol{V} = \boldsymbol{I}_k} \operatorname{tr}(\boldsymbol{V}^\top \boldsymbol{C}\boldsymbol{S}^\top \boldsymbol{S}\boldsymbol{C}^\top \boldsymbol{V}) = \min_{\boldsymbol{V}^\top \boldsymbol{V} = \boldsymbol{I}_k} \|\boldsymbol{S}\boldsymbol{C}^\top \boldsymbol{V}\|_F^2$$

Set $\boldsymbol{Z} = \boldsymbol{C}\boldsymbol{U}_{k_1}$, and suppose that $\boldsymbol{Z}^\top \boldsymbol{Z}$ is invertible (this will be ensured in the following). We select

$$\boldsymbol{V} = \boldsymbol{Z}(\boldsymbol{Z}^\top \boldsymbol{Z})^{-1/2}$$

for which we have

$$\boldsymbol{V}^\top \boldsymbol{V} = (\boldsymbol{Z}^\top \boldsymbol{Z})^{-1/2} \boldsymbol{Z}^\top \boldsymbol{Z} (\boldsymbol{Z}^\top \boldsymbol{Z})^{-1/2} = \boldsymbol{I}_{k_1}$$

as required.

We expand the sum of eigenvalues as follows:

$$\sum_{i\le k_1} \boldsymbol{\lambda}_i = \min_{\boldsymbol{V}^\top \boldsymbol{V} = \boldsymbol{I}_{k_1}} \|\boldsymbol{S}\boldsymbol{C}^\top \boldsymbol{V}\|_{\boldsymbol{F}}^2 \le \|\boldsymbol{S}\boldsymbol{C}^\top \boldsymbol{Z}(\boldsymbol{Z}^\top \boldsymbol{Z})^{-1/2}\|_F^2 \le \|\boldsymbol{S}\boldsymbol{C}^\top \boldsymbol{C}\boldsymbol{U}_{k_1}\|_F^2 \, \|(\boldsymbol{Z}^\top \boldsymbol{Z})^{-1/2}\|_2^2.$$

and use the matrix $\boldsymbol{\Pi} = \boldsymbol{C}^\top \boldsymbol{C}$ and $\boldsymbol{\Pi}^\perp = \boldsymbol{I} - \boldsymbol{\Pi}$ defined in Section 3.2.

For the first term, we employ the triangle inequality.

$$\begin{aligned} \|\boldsymbol{S}\boldsymbol{C}^\top \boldsymbol{C}\boldsymbol{U}_{k_1}\|_F^2 &= \|\boldsymbol{S}\boldsymbol{\Pi}\boldsymbol{U}_{k_1}\|_F^2 \\ &= (\|\boldsymbol{S}(\boldsymbol{I} - \boldsymbol{\Pi}^\perp)\boldsymbol{U}_{k_1}\|_F)^2 \\ &\le (\|\boldsymbol{S}\boldsymbol{U}_{k_1}\|_F + \|\boldsymbol{S}\boldsymbol{\Pi}^\perp \boldsymbol{U}_{k_1}\|_F)^2 \\ &\le (\|\boldsymbol{S}\boldsymbol{U}_{k_1}\|_F + \|\boldsymbol{S}\boldsymbol{\Pi}^\perp\|_2 \|\boldsymbol{\Pi}^\perp \boldsymbol{U}_{k_1}\|_F)^2 \end{aligned} \tag{5}$$

The result for $\|\boldsymbol{S}\boldsymbol{U}_{k_1}\|_F$ is

$$\|\boldsymbol{S}\boldsymbol{U}_{k_1}\|_F = \sqrt{\mathrm{tr}(\boldsymbol{U}_{k_1}^\top \boldsymbol{S}^\top \boldsymbol{S}\boldsymbol{U}_{k_1})} = \sqrt{\sum_{i\le k_1} \boldsymbol{\lambda}(i)}.$$

On the other hand, the norm $\|\boldsymbol{S}\boldsymbol{\Pi}^\perp\|_2$ is bounded by

$$\|\boldsymbol{S}\boldsymbol{\Pi}^\perp\|_2 = \sqrt{\lambda_{\max}(\boldsymbol{\Pi}^\perp \boldsymbol{S}^\perp \boldsymbol{S}\boldsymbol{\Pi}^\perp)} = \sqrt{\lambda_{\max}(\boldsymbol{\mathcal{L}})} \le \sqrt{2}$$

To analyze the second term, denote by σ_i the singular values of the $k\times k$ matrix $\boldsymbol{U}_{k_1}^\top \boldsymbol{\Pi}\boldsymbol{U}_{k_1}$ and $\delta_{k_1} = \mathcal{F}(\boldsymbol{U}_{k_1}, C) = \|\boldsymbol{\Pi}^\perp \boldsymbol{U}_{k_1}\|_F^2$. The following inequality holds:

$$\delta_{k_1} \ge \|\boldsymbol{\Pi}^\perp \boldsymbol{U}_{k_1}\|_2^2 = \|\boldsymbol{U}_{k_1}^\top \boldsymbol{\Pi}^\perp \boldsymbol{\Pi}^\perp \boldsymbol{U}_{k_1}\|_2 = \|\boldsymbol{U}_{k_1}^\top \boldsymbol{\Pi}^\perp \boldsymbol{U}_{k_1}\|_2 = \|\boldsymbol{U}_{k_1}^\top (\boldsymbol{I}-\boldsymbol{\Pi})\boldsymbol{U}_{k_1}\|_2 = \|\boldsymbol{I}_k - \boldsymbol{U}_{k_1}^\top \boldsymbol{\Pi}\boldsymbol{U}_{k_1}\|_2$$

The inequality is equivalent to asserting that the singular values of $\boldsymbol{U}_{k_1}^\top \boldsymbol{\Pi}\boldsymbol{U}_{k_1}$ are concentrated around one, i.e.,

$$1-\delta_{k_1} \le \sigma_i \le 1+\delta_{k_1} \quad \text{for all} \quad i \le k_1.$$

It follows that the smallest eigenvalue of the PSD matrix $\boldsymbol{Z}^\top \boldsymbol{Z}$ is bounded by

$$\begin{aligned}
\boldsymbol{\lambda}_1(\boldsymbol{Z}^\top \boldsymbol{Z}) &= \min_{\|\boldsymbol{x}\|_2=1} x^\top \boldsymbol{U}_{k_1}^\top \boldsymbol{C}^\top \boldsymbol{C}\boldsymbol{U}_{k_1}\boldsymbol{x} \\
&= \min_{\boldsymbol{x}\in\mathrm{span}(\boldsymbol{U}_{k_1}),\ \|\boldsymbol{x}\|_2=1} x^\top \boldsymbol{C}^\top \boldsymbol{C} x \\
&= \min_{\boldsymbol{x}\in\mathrm{span}(\boldsymbol{U}_{k_1}),\ \|\boldsymbol{x}\|_2=1} \boldsymbol{x}^\top \boldsymbol{\Pi} x \\
&\ge 1-\delta_{k_1}
\end{aligned}$$

We deduce that the matrix is invertible when $\delta_{k_1} < 1$ and $\boldsymbol{C}$ is full row-rank. In addition, we have

$$\|(\boldsymbol{Z}^\top \boldsymbol{Z})^{-1/2}\|_2^2 = \|(\boldsymbol{Z}^\top \boldsymbol{Z})^{-1}\|_2 \le \frac{1}{1-\delta_{k_1}}.$$

Putting the bounds together, gives

$$\sum_{i\le k_1} \boldsymbol{\lambda}_c(i) \le \frac{\left(\sqrt{\sum_{i\le k}\boldsymbol{\lambda}(i)} + \sqrt{2\,\delta_{k_1}}\right)^2}{1-\delta_{k_1}}$$

or equivalently

$$\sum_{i\le k}(\boldsymbol{\lambda}_c(i) - \boldsymbol{\lambda}(i)) \le \frac{\left(\sqrt{\sum_{i\le k}\boldsymbol{\lambda}(i)} + \sqrt{2\,\delta_{k_1}}\right)^2}{1-\delta_{k_1}} - \sum_{i\le k_1}\boldsymbol{\lambda}(i) = \frac{\delta_{k_1}(2+\sum_{i\le k}\boldsymbol{\lambda}(i)) + \sqrt{8\delta_{k_1}\sum_{i\le k_1}\boldsymbol{\lambda}(i)}}{1-\delta_{k_1}}$$

To prove the result for the second term in equation 4, we introduce the *signless normalized Laplacian* $\tilde{\boldsymbol{\mathcal{L}}} = \boldsymbol{I} + \boldsymbol{D}^{-1/2}\boldsymbol{W}\boldsymbol{D}^{-1/2}$ to obtain the results of the second term in Equation. 5. We follow the similar arguments using the signless normalized Laplacian. Note that the spectral properties of signless normalized Laplacian follow the relation:

$$\tilde{\boldsymbol{\lambda}}(i) = 2 - \boldsymbol{\lambda}(N+1-i) \text{ and } \tilde{\boldsymbol{U}}(i) = \boldsymbol{U}(N+1-i)$$

Then, the eigengaps between largest eigenvalues abide to

$$\begin{aligned}
\sum_{j=k_2+1}^{N}(\boldsymbol{\lambda}(j) - \boldsymbol{\lambda}_c(j+n-N)) &= \sum_{j=1}^{n-k}\boldsymbol{\lambda}(N+1-j) - \boldsymbol{\lambda}_c(n+1-j) \\
&= \sum_{j=1}^{n-k}(\tilde{\boldsymbol{\lambda}}_c(j) - \tilde{\boldsymbol{\lambda}}(j)) \\
&\le \frac{\delta'_{k_2}(\sum_{j\le n-k_1} 2 + \tilde{\boldsymbol{\lambda}}(j)) + \sqrt{8\delta'_{k_2}\sum_{j\le n-k_1}\tilde{\boldsymbol{\lambda}}(j)}}{1-\delta'_{k_2}}.
\end{aligned}$$

Combining the above, we obtain the following result:

$$\begin{aligned} SD(\mathcal{G}, \mathcal{G}_c) &\leq \frac{\delta_{k_1}(2 + \sum_{i \leq k} \boldsymbol{\lambda}(i)) + \sqrt{8\delta_{k_1} \sum_{i \leq k_1} \boldsymbol{\lambda}(i)}}{1 - \delta_{k_1}} + \frac{\delta'_{k_2}(\sum_{j \leq n-k_1} 2 + \tilde{\boldsymbol{\lambda}}(j)) + \sqrt{8\delta'_{k_2} \sum_{j \leq n-k_1} \tilde{\boldsymbol{\lambda}}(j)}}{1 - \delta'_{k_2}} \\ &\leq \frac{(n+2)\mathcal{F}(\boldsymbol{U}, \boldsymbol{C}) + 4\sqrt{\mathcal{F}(\boldsymbol{U}, \boldsymbol{C})}}{1 - \mathcal{F}(\boldsymbol{U}, \boldsymbol{C})} \end{aligned}$$

In the last step, we use the following bounds:

$$\delta_{k_1} \leq \mathcal{F}(\boldsymbol{U}, \boldsymbol{C}), \delta'_{k_2} \leq \mathcal{F}(\boldsymbol{U}, \boldsymbol{C}),$$
$$\sum_{i \leq k_1} \boldsymbol{\lambda}(i) \leq k_1, \sum_{j \leq n-k_1} \tilde{\boldsymbol{\lambda}}(j) \leq n - k_1$$
$$\sqrt{k_1} + \sqrt{n - k_1} \leq \sqrt{2n}.$$

□

E Additional Material for Experiments

E.1 Graph Classification Dataset

The statistics of the graph classification benchmarks are in Table 1.

Table 1: Statistics of the graph benchmark datasets.

Datasets	**MUTAG**	**ENZYMES**	**NCI1**	**NCI109**	**PROTEINS**	**PTC**
Sample size	188	600	4110	4127	1108	344
Average $\lvert V \rvert$	17.93	32.63	29.87	29.68	39.06	14.29
Average $\lvert E \rvert$	19.79	62.14	32.3	32.13	72.70	14.69
# classes	2	6	2	2	2	2

E.2 Definition of Normalized Mutual Information

We denote C_1 and C_2 are two where $C(i)$ represents the set of nodes with label i. We define the NMI as,

$$NMI(C_1, C_2) = \frac{MI(C_1, C_2)}{\frac{1}{2}(H(C_1) + H(C_2))}$$

where $MI(C_1, C_2)$ is the mutual information defined as,

$$MI(C_1, C_2) = \sum_{i=1}^{n} \sum_{j=1}^{n} p(C_1(i) \cap C_2(j)) \log \left(\frac{p\left(C_1(i) \cap C_2(j)\right)}{p\left(C_1(i)\right) p\left(C_2(j)\right)} \right)$$

$H(C)$ is the entropy defined as,

$$H(C) = -\sum_{i=1}^{n} p(C(i)) \log p(C(i))$$

The probability $p(C(i))$ is approximated as the ratio of partition i as $p(C(i)) = \frac{|C(i)|}{N}$.

References

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