

A Proof of Lemma 4.2

The regularization is:

$$\begin{aligned}
\sum_{i=1}^N \sum_{j=1}^N \|C_i - C_j\|_2^2 &= \sum_{i=1}^N \sum_{j=1}^N (C_i^T C_i - 2C_i^T C_j + C_i^T C_i) \\
&= 2N \sum_{i=1}^N C_i^T C_i - 2 \sum_{i=1}^N \sum_{j=1}^N C_i^T C_j \\
&= 2N \sum_{i=1}^N C_i^T (C_i - \frac{1}{N} \sum_{j=1}^N C_j) = 2N \sum_{i=1}^N C_i^T (C_i - \bar{C}) \\
&\stackrel{(*)}{=} 2N \sum_{i=1}^N \|C_i - \bar{C}\|_2^2,
\end{aligned} \tag{21}$$

where $(*)$ derives from the equality $\sum_{i=1}^N \bar{C}^T (C_i - \bar{C}) = 0$. Hence, the regularization is used to maximize the sample variance. Assume that only samples are accessible to the target distribution $\text{Dir}(\beta)$, we consider the variance instead (i.e., $\mathbb{E}_{C_i \sim \text{Dir}(\beta)} [\sum_{i=1}^N \|C_i - \bar{C}\|_2^2]$). To simplify the notation (i.e., ignore the constant),

$$\mathbb{E}_{x \sim \text{Dir}(\beta)} [(x - \mathbb{E}[x])^T (x - \mathbb{E}[x])] = \sum_{k=1}^K \text{Var}(x_k) = \sum_{k=1}^K \frac{\beta_k(\beta_0 - \beta_k)}{\beta_0^2(\beta_0 + 1)}. \tag{22}$$

Here, we have $\beta_0 = \sum_{k=1}^K \beta_k$. We want to investigate the effect of adding this regularization w.r.t. to parameter β . Alternatively, we consider the optimization problem as below,

$$\begin{aligned}
&\max_{\beta} \sum_{k=1}^K \frac{\beta_k(\beta_0 - \beta_k)}{\beta_0^2(\beta_0 + 1)} \\
&\text{s.t. } \beta_k \geq 0, \forall k \in [K].
\end{aligned} \tag{23}$$

Then, we have $t^* = \sum_{k=1}^K \beta_k^*$ where β^* is the optimal point. We take a step towards the following convex problem,

$$\begin{aligned}
&\min_{\beta} - \sum_{k=1}^K \beta_k (t^* - \beta_k) \\
&\text{s.t. } \sum_{k=1}^K \beta_k = t^*, \\
&\quad \beta_k \geq 0, \forall k \in [K].
\end{aligned} \tag{24}$$

As the Slater condition holds, KKT condition is necessary and sufficient. The so-called augmented Lagrangian function is

$$L(\beta, \nu, \pi) = - \sum_{k=1}^K \beta_k (t^* - \beta_k) + \nu (\sum_{k=1}^K \beta_k - t^*) - \sum_{k=1}^K \pi_k \beta_k.$$

The KKT condition is

$$\begin{cases} -t^* + 2\beta_k + \nu - \pi_k = 0, \forall k \in [K] \\ \sum_{k=1}^K \beta_k - t^* = 0, \\ \pi_k \beta_k = 0, \beta_k \geq 0, \pi_k \geq 0 \forall k \in [K] \end{cases} \tag{25}$$

Consider the case $\pi_k = 0, \beta_k > 0$, we have $\beta_k^* = \frac{t^*}{K}, \nu^* = \frac{K-2}{K} t^*$. We come back to the original problem,

$$\sum_{k=1}^K \frac{\beta_k(\beta_0 - \beta_k)}{\beta_0^2(\beta_0 + 1)} = \frac{K-1}{K t^*}.$$

Overall, maximizing this component enforces $t^* \rightarrow 0$ and all equal parameters for the Dirichlet distributions.

B Proof of Proposition 5.1

The distance between an arbitrary spectral filter $g(\lambda)$ and the ideal *low pass* filter $g_{\text{id}}(\lambda)$ in Eq. 4 is defined as,

$$\text{Distance}(g, g_{\text{id}}) = \int_0^{\lambda_K} (1 - g(\lambda))^2 d\lambda + \int_{\lambda_K}^2 (0 - g(\lambda))^2 d\lambda. \tag{26}$$

Intuitively, this definition computes the squared Euclidean distance between $g(\cdot)$ and $g_{id}(\cdot)$. Thus, the distance between GCN $g_c(\cdot)$ and the ideal low pass $g_{id}(\cdot)$ is:

$$\begin{aligned} \text{Distance}(g_c, g_{id}) &= \int_0^{\lambda_K} (1 - (1 - \lambda))^2 d\lambda + \int_{\lambda_K}^2 (0 - (1 - \lambda))^2 d\lambda \\ &= \lambda_K^2 - \lambda_K + \frac{2}{3} \end{aligned} \quad (27)$$

The distance between Heatts $g_s(\cdot)$ and the ideal low pass $g_{id}(\cdot)$:

$$\text{Distance}(g_s, g_{id}) = \int_0^{\lambda_K} (-s\lambda + \frac{1}{2}s^2\lambda^2 - \frac{1}{6}s^3\lambda^3)^2 d\lambda + \int_{\lambda_K}^2 (1 - s\lambda + \frac{1}{2}s^2\lambda^2 - \frac{1}{6}s^3\lambda^3)^2 d\lambda \quad (28)$$

Our purpose is to derive value range of s such that $\text{Distance}(g_s, g_{id})$ is always smaller than $\text{Distance}(g_c, g_{id})$.

$$\text{Distance}(g_s, g_{id}) - \text{Distance}(g_c, g_{id}) \geq 0 \quad (29)$$

The solution is $0.672 \leq s \leq 1.321$

As shown in Figure 4, Heatts is always closer to the ideal low pass $g_{id}(\cdot)$ when $s \in [0.672, 1.321]$.

Table 3: Statistics of data sets used in graph clustering

Data	Nodes	Edges	Classes	features
Pubmed	19,717	44,338	3	500
Citeseer	3,327	4,732	6	3,703
Wiki	2,405	17,981	17	4,973

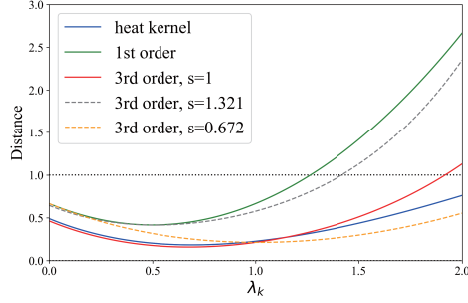


Figure 4: The distance between spectral filters and the ideal low pass