Exercise: Spectral Clustering (2 Points)

Assume the graph is connected.

Let $G = (V, E, W)$ be a weighted, undirected, connected graph with weight matrix $W = (w_{ij})$, degree matrix $D = \mathrm{diag}(d_1, \ldots, d_n)$ where $d_i = \sum_j w_{ij}$, and (unnormalized) Laplacian $L = D - W$. Consider the optimization problem

$$\min_{F \in \mathbb{R}^{n \times k}} \quad \sum_{(i,j) \in E} w_{ij} \, \|f(i) - f(j)\|^2$$
$$\text{s.t.} \quad F^\top F = I_k, \qquad F^\top \mathbf{1}_n = 0,$$

where $F = [f_1, \ldots, f_k]$ and $f(i) \in \mathbb{R}^k$ denotes the i-th row of F.

Theorem 1. *Let $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ be the eigenvalues of L, with corresponding orthonormal eigenvectors $u_1, \ldots, u_n$, and $u_1 = \frac{1}{\sqrt{n}} \mathbf{1}_n$. The optimal solution of*

$$\min_{F \in \mathbb{R}^{n \times k}} \sum_{(i,j) \in E} w_{ij} \|f(i) - f(j)\|^2 \quad \text{subject to } F^\top F = I_k, \ F^\top \mathbf{1}_n = 0$$

is achieved by

$$F^\star = \left[\, u_2, \ u_3, \ \ldots, \ u_{k+1} \,\right],$$

i.e., the columns of $F^\star$ are the eigenvectors of L associated with $\lambda_2, \ldots, \lambda_{k+1}$.

Proof. **Step 1: Matrix form of the objective.** For any vector $f \in \mathbb{R}^n$,

$$\sum_{i,j} w_{ij} \, (f_i - f_j)^2 \; = \; 2 \, f^\top L f.$$

Applying this to each column f_ℓ of $F = [f_1, \ldots, f_k]$ and summing over ℓ yields

$$\sum_{i,j} w_{ij} \, \|f(i) - f(j)\|^2 \; = \; 2 \sum_{\ell=1}^{k} f_\ell^\top L f_\ell \; = \; 2 \, \mathrm{Tr}\Big(F^\top L F\Big).$$

Thus the problem is equivalent to

$$\min_{F \in \mathbb{R}^{n \times k}} \mathrm{Tr}\Big(F^\top L F\Big) \quad \text{s.t. } F^\top F = I_k, \ F^\top \mathbf{1}_n = 0.$$

Step 2: Spectral decomposition. Since L is real, symmetric, and positive semidefinite, there exists an orthonormal eigenbasis $U = [u_1, \ldots, u_n]$ with $LU = U\Lambda$, $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$, and (because the graph is connected) $\lambda_1 = 0$ with $u_1 = \frac{1}{\sqrt{n}} \mathbf{1}_n$. Express F in this basis:

$$F \; = \; UA, \qquad A \in \mathbb{R}^{n \times k}.$$

Then

$$\mathrm{Tr}\Big(F^\top L F\Big) \; = \; \mathrm{Tr}(A^\top U^\top L U A) \; = \; \mathrm{Tr}(A^\top \Lambda A) \; = \; \sum_{i=1}^{n} \lambda_i \, \|a_i\|^2,$$

where $a_i^\top$ is the i-th row of A.

Step 3: Constraints in eigenbasis. From $F^\top F = I_k$ we get

$$A^\top A = I_k \;\; \Rightarrow \;\; \sum_{i=1}^{n} \|a_i\|^2 = k.$$

From $F^\top \mathbf{1}_n = 0$ and $U^\top \mathbf{1}_n = \sqrt{n}\, e_1$ we get

$$0 = F^\top \mathbf{1}_n = A^\top U^\top \mathbf{1}_n = \sqrt{n}\, A^\top e_1 \quad \Rightarrow \quad a_1 = 0.$$

Hence the entire "mass" $\sum_i \|a_i\|^2 = k$ must be distributed among rows $i \geq 2$.

Step 4: Minimization. The objective

$$\mathrm{Tr}\Big(A^\top \Lambda A\Big) = \sum_{i=1}^{n} \lambda_i \|a_i\|^2$$

is minimized, subject to $A^\top A = I_k$ and $a_1 = 0$, by allocating the k orthonormal rows of A to the *smallest* available eigenvalues, i.e., to indices $i = 2, \ldots, k+1$. Concretely, take A so that its columns are the standard basis vectors $e_2, \ldots, e_{k+1}$ (up to any $k \times k$ orthogonal rotation), which implies

$$F = UA = [u_2, \ldots, u_{k+1}]\, Q$$

for some $Q \in \mathbb{R}^{k \times k}$ orthogonal. Since $F^\top F = I_k$ and the objective is invariant under right multiplication by Q, we can take $Q = I_k$ without loss of generality. Thus an optimal solution is

$$F^\star = [u_2, \ldots, u_{k+1}],$$

achieving the minimum value $\sum_{\ell=2}^{k+1} \lambda_\ell$. □

Remark. The eigenvector $u_1 \propto \mathbf{1}_n$ (corresponding to $\lambda_1 = 0$) is excluded by the constraint $F^\top \mathbf{1}_n = 0$. Hence the solution uses the next k eigenvectors, $u_2, \ldots, u_{k+1}$.