Ruben Cardoso
ruben.cardoso@dauphine.eu

Lab Session 4
ALTEGRAD 2025

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QUESTION 1

The graph G consists of two connected components: a complete graph K_{20} and a complete bipartite graph $K_{10,10}$. Therefore, G has $20 + 20 = 40$ vertices in total.
We analyze the structure of the complement graph $\overline{G}$.

- K_{20}, every possible edge exists in G, hence none exists in $\overline{G}$. Thus, these 20 vertices form an independent set in $\overline{G}$.

- In $K_{10,10}$, edges exist only across the two sets of size 10. Therefore, in $\overline{G}$, all edges appear within each part, forming two disjoint cliques K_{10} and K_{10}, while there are no edges between the two parts.

- Since the two components of G are disconnected, there are no edges between K_{20} and $K_{10,10}$ in G. Hence, in $\overline{G}$, all possible edges appear between these sets, forming a complete bipartite structure between the 20 vertices of K_{20} and the 20 vertices of $K_{10,10}$.

Thus, triangles in $\overline{G}$ may only occur in the following situations:

1. Three vertices inside one of the K_{10} cliques:
$$2 \times \binom{10}{3} = 2 \times 120 = 240.$$
2. One vertex from K_{20} and two vertices from one K_{10} clique:
$$2 \times \left(20 \times \binom{10}{2}\right) = 2 \times (20 \times 45) = 1800.$$

Adding all contributions gives:

$$\Delta(\overline{G}) = 240 + 1800 = 2040.$$

where Δ gives returns the number of triangle for any undirected graph.

QUESTION 2

Let $A \in \mathbb{R}^{n \times n}$ be a symmetric adjacency matrix and consider the Rayleigh quotient

$$R(A, x) = \frac{x^\top A x}{x^\top x}, \qquad x \neq 0.$$

Define

$$u(x) = x^\top A x \quad \text{and} \quad v(x) = x^\top x,$$

so that $R(A, x) = \dfrac{u(x)}{v(x)}$.

Since A is symmetric, the gradient of u satisfies

$$\nabla u(x) = 2Ax,$$

and the gradient of v satisfies

$$\nabla v(x) = 2x.$$

Applying the quotient rule for gradients,

$$\nabla R(A,x) = \frac{v(x)\,\nabla u(x) - u(x)\,\nabla v(x)}{(v(x))^2} = \frac{2(x^\top x)Ax - 2(x^\top Ax)x}{(x^\top x)^2}.$$

Thus, $\nabla R(A,x) = 0$ if and only if

$$(x^\top x)Ax = (x^\top Ax)x.$$

Since $R(A,x) \in \mathbb{R}$ and :

$$Ax = R(A,x)\,x,$$

Thus x is necessarily an eigenvector of A of associated eigen value $R(A,x)$.

Conversely, if x is an eigenvector of A, say $Ax = \lambda x$, for some real value λ, then

$$R(A,x) = \frac{x^\top(\lambda x)}{x^\top x} = \lambda,$$

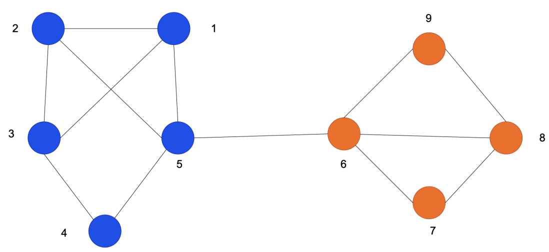
a constant. Its gradient is therefore zero, which proves that x is a stationary point of $R(A,\cdot)$. Recall that an eigenvector is never 0 so $x^\top x$ never vanishes if x is an eigenvector.

QUESTION 3

We recall the modularity formula:

$$Q = \sum_{c=1}^{n_c} \left[\frac{l_c}{m} - \left(\frac{d_c}{2m} \right)^2 \right],$$

Let us first start with Graph (a).



(a)

Figure 1:

Based on our manual count:

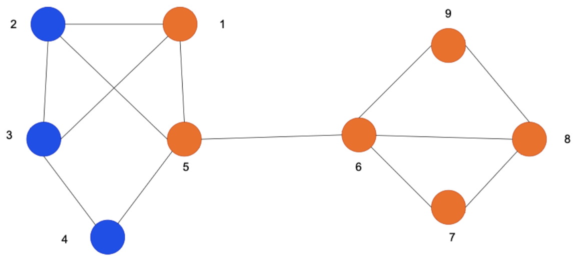
- $m = 13$
- $l_1^a = 7 \quad$ (internal blue edges)
- $l_2^a = 5 \quad$ (internal orange edges)

- $d_1^a = 15$ (total degree of blue community)
- $d_2^a = 11$ (total degree of orange community)

Thus,

$$Q_a = \left(\frac{7}{13} - \left(\frac{15}{26}\right)^2\right) + \left(\frac{5}{13} - \left(\frac{11}{26}\right)^2\right) \approx 0.412.$$

Now for graph (b) :



(b)

Figure 2:

Based on the second assignment:

- $l_1^b = 2$
- $l_2^b = 7$
- $d_1^b = 8$
- $d_2^b = 18$

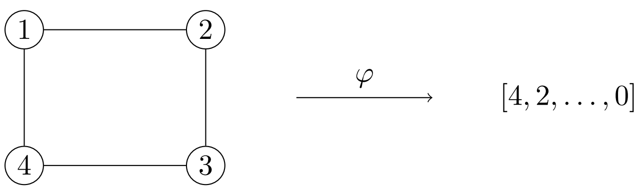
Therefore,

$$Q_b = \left(\frac{2}{13} - \left(\frac{8}{26}\right)^2\right) + \left(\frac{7}{13} - \left(\frac{18}{26}\right)^2\right) \approx 0.119.$$

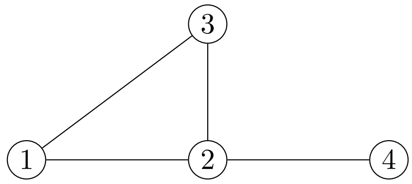
Both Q_a and Q_b are positive, indicating that in both cases the partitions exhibit more community structure than what would be expected at random given the degree sequence. However and as expected, $Q_a \approx 0.412$ is more than 3 times higher than $Q_b \approx 0.119$, showing that the assignment in graph (a) yields a much stronger and more clearly separated community structure compared to graph (b).

QUESTION 4:

Let φ be the shortest path kernel function that maps a graph G to a sequence $\varphi(G) = (c_1, \dots, c_D)$, where D is the graph diameter and c_i denotes the total number of shortest paths of length i in G. Hence, each coordinate c_i of the feature sequence counts how many distinct pairs of vertices in G are connected by a shortest path of length i.



$G^{(1)}$



$$\xrightarrow{\varphi} \quad [4, 2, \ldots, 0]$$

$G^{(2)}$

Whence :

$$\varphi(G^{(1)}) = \varphi(G^{(2)}) \qquad \text{but} \qquad G^{(1)} \not\simeq G^{(2)}$$

Remark: The *shortest path kernel* is not "injective" in the sense that two non-isomorphic graphs can be mapped to the same feature vector representation.

Question 5

We apply one iteration of the 1-dimensional Weisfeiler–Lehman (WL) subtree refinement to the two labeled graphs G and G' of Figure 5. Initially, each node keeps its given numerical label in $\{1, \ldots, 5\}$. For each vertex v, the new color is defined as:

$$\text{new\_label}(v) = \text{hash}\big(\text{label}(v) \mid \{\text{label}(u) : u \in N(v)\}\big),$$

where the hash function only needs to be injective. We denote distinct hash outputs abstractly as $c_A, c_B, \ldots$.

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Graph G (left) We distinguish the two vertices labeled 1 as 1_{top} and 1_{bot}.

- 2: $\text{hash}(2 \mid \{1, 3, 4, 5\}) = c_A$
- 1_{top}: $\text{hash}(1 \mid \{2, 5\}) = c_B$
- 5: $\text{hash}(5 \mid \{1, 2, 3\}) = c_C$
- 4: $\text{hash}(4 \mid \{1, 2, 3\}) = c_D$
- 3: $\text{hash}(3 \mid \{1, 2, 4, 5\}) = c_E$
- 1_{bot}: $\text{hash}(1 \mid \{3, 4\}) = c_F$

Thus, the multiset of WL colors after one iteration is:

$$\mathcal{C}_G^{(1)} = \{c_A, c_B, c_C, c_D, c_E, c_F\}.$$

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Graph G' (right) Since two vertices have initial label 4, we write 4_{L} and 4_{R}.

- 2: $\text{hash}(2 \mid \{1, 4, 5\}) = c_G$
- 1: $\text{hash}(1 \mid \{2, 5\}) = c_B$ (same as in graph G)
- 5: $\text{hash}(5 \mid \{1, 2, 4\}) = c_H$
- 4_{L}: $\text{hash}(4 \mid \{2, 3\}) = c_I$
- 4_{R}: $\text{hash}(4 \mid \{3, 5\}) = c_J$

- 3: $\mathrm{hash}(3 \mid \{4, 4\}) = c_K$

Thus,

$$\mathcal{C}_{G'}^{(1)} = \{c_G, c_B, c_H, c_I, c_J, c_K\}.$$

—

Only one color matches across both graphs, namely c_B. Therefore, the WL kernel after one iteration equals:

$$k(G, G') = |\mathcal{C}_G^{(1)} \cap \mathcal{C}_{G'}^{(1)}| = 1.$$

This indicates **very weak structural similarity** once neighborhood information is incorporated: the two graphs become almost completely distinguishable after a single WL refinement.