ALTEGRAD Lab 4 questions

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Question 1. We consider the structure of the complement graph. In the original graph, the component on 20 vertices is a complete graph, so in the complement graph no edges exist between these 20 vertices. The other component is a complete bipartite graph $K_{10,10}$, meaning that in the complement graph each part of size 10 becomes a complete graph K_{10} and no edges appear between the two parts.

First, we count triangles entirely inside the two K_{10} components of the complement graph. Each K_{10} contains $\binom{10}{3} = 120$ triangles. Since there are two such components, this contributes $2 \times 120 = 240$ triangles.

Next, we count triangles formed by taking one vertex from the independent set of 20 vertices and two vertices from the same K_{10} component. Each K_{10} contains $\binom{10}{2} = 45$ pairs of vertices, and for each of the 20 vertices in the independent set, each of these pairs forms a triangle. Since there are two K_{10} components, this contributes $20 \times 2 \times 45 = 1800$ triangles.

Adding the two, the total number of triangles in the complement graph is

$$240 + 1800 = 2040.$$

Question 2. We prove the equivalence in two directions.

First direction. If $x \neq 0$ is a stationary point of

$$R(A, x) = \frac{x^T Ax}{x^T x},$$

then its gradient is equal to 0. Using the usual gradients $\nabla(x^T Ax) = 2Ax$ and $\nabla(x^T x) = 2x$ and the quotient rule for gradients, we get

$$\begin{aligned}
\nabla R(A, x) &= \frac{2Ax\,(x^T x) - 2x\,(x^T Ax)}{(x^T x)^2} = 0 \\
&\implies 2Ax\,(x^T x) - 2x\,(x^T Ax) = 0 \\
&\implies Ax\,(x^T x) - x\,(x^T Ax) = 0 \\
&\implies (x^T x)\,Ax - (x^T Ax)\,x = 0 \\
&\implies Ax - \frac{x^T Ax}{x^T x}\,x = 0 \qquad (x^T x \neq 0) \\
&\implies Ax = \left(\frac{x^T Ax}{x^T x}\right) x.
\end{aligned}$$

Since $x^T x \neq 0$, set $\lambda = \dfrac{x^T Ax}{x^T x}$. The previous equality is equivalent to $Ax = \lambda x$, so x is an eigenvector of A.

Second direction. Conversely, if $Ax = \lambda x$ for some scalar λ, then $\nabla(x^T Ax) = 2Ax = 2\lambda x$ and $\nabla(x^T x) = 2x$. Substituting into the gradient formula gives

$$\nabla R(A, x) = \frac{2\lambda x\,(x^T x) - 2x\,(\lambda x^T x)}{(x^T x)^2} = 0,$$

so the gradient vanishes and x is a stationary point of $R(A, \cdot)$.

Therefore a non-zero vector x is a stationary point of the Rayleigh quotient if and only if it is an eigenvector of A.

Question 3. For figure (a): The graph has $m = 13$ edges in total. There are $n_c = 2$ clusters.

For cluster 1 (blue):

$$\ell_{\text{blue}} = 7, \qquad d_{\text{blue}} = 3 + 3 + 3 + 2 + 4 = 15$$

For cluster 2 (orange):

$$\ell_{\text{orange}} = 5, \qquad d_{\text{orange}} = 4 + 2 + 2 + 3 = 11$$

The modularity is computed as:

$$Q_a = \sum_{c=1}^{2} \left(\frac{\ell_c}{m} - \left(\frac{d_c}{2m} \right)^2 \right) = \left(\frac{7}{13} - \left(\frac{15}{26} \right)^2 \right) + \left(\frac{5}{13} - \left(\frac{11}{26} \right)^2 \right)$$

Therefore, the modularity for figure (a) is $\mathrm{Q}_a \approx 0.411$.

For figure (b): The graph has $m = 13$ edges in total. There are $n_c = 2$ clusters.

For cluster 1 (blue):

$$\ell_{\text{blue}} = 2, \qquad d_{\text{blue}} = 3 + 3 + 2 = 8$$

For cluster 2 (orange):

$$\ell_{\text{orange}} = 7, \qquad d_{\text{orange}} = 4 + 3 + 4 + 2 + 2 + 3 = 18$$

The modularity is computed as:

$$Q_b = \sum_{c=1}^{2} \left(\frac{\ell_c}{m} - \left(\frac{d_c}{2m} \right)^2 \right) = \left(\frac{2}{13} - \left(\frac{8}{26} \right)^2 \right) + \left(\frac{7}{13} - \left(\frac{18}{26} \right)^2 \right)$$

Therefore, the modularity for figure (b) is $\mathrm{Q}_b \approx 0.118$.

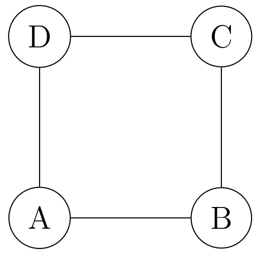
Modularity measures the quality of a partition: higher values indicate that nodes within the same cluster are more densely connected, and there are fewer edges between clusters.

Since Q_a is significantly higher than Q_b, the partition in figure (a) better reflects the community structure of the graph.

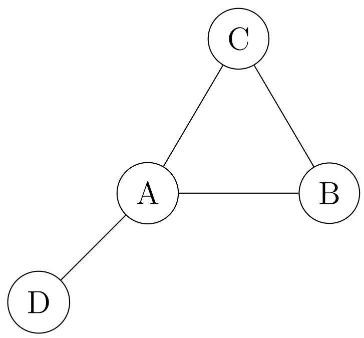
Therefore, the partition of figure (a) is considered better than that of figure (b).

Question 4. We provide an example of two non-isomorphic graphs that are mapped to the same representation by the shortest path kernel.

Graph 1:



Graph 2:



The two graphs are not isomorphic. In Graph 1, all four nodes have degree 2. In Graph 2, one node has degree 3, one has degree 1, and the remaining two have degree 2. Since isomorphic graphs must have identical degree distributions, these two graphs cannot be isomorphic.

The shortest path kernel represents a graph by counting, for every pair of nodes, the length of the shortest path between them.

- Both graphs have exactly 4 nodes.
- They have the same number of shortest paths of length 1. In each graph there are 4 shortest paths of length 1:

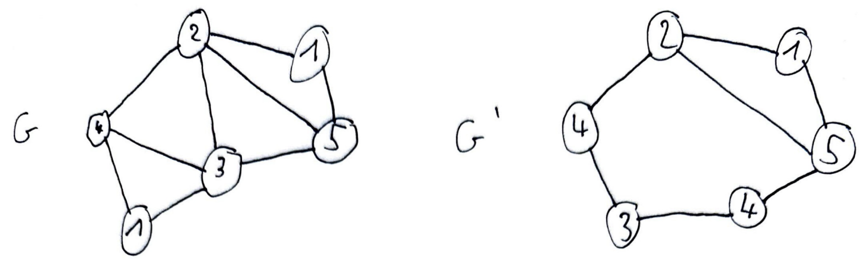
$$A-B, \quad B-C, \quad C-D, \quad D-A.$$

- They also have the same number of shortest paths of length 2. In each graph there are 2 shortest paths of length 2:

$$A-C \text{ via } B, \qquad B-D \text{ via } A.$$

- Neither graph contains shortest paths longer than 2.

Therefore, the shortest path kernel maps both graphs to the same feature representation, despite the fact that they are not isomorphic.



G	G'
$1 \to 1,25$	$1 \to 1,25$
$1 \to 1,34$	$2 \to 2,145$
$2 \to 2,1345$	$3 \to 3,44$
$3 \to 3,1245$	$4 \to 4,23$
$4 \to 4,123$	$4 \to 4,35$
$5 \to 5,123$	$5 \to 5,124$

Before relabeling, (step 0):

$$\langle \phi_0(G), \phi_0(G') \rangle = 2\times1 + 1\times1 + 1\times1 + 1\times2 + 1\times1 = 7$$

After relabeling, (step 1):

$\langle \phi_1(G), \phi_1(G') \rangle = 1$ (only 1 common color)

Indeed, $K_{WL}(G, G') = 7 + 1 = 8$.

Figure 1: One iteration of the WL algorithm

Question 5. Here is what we obtain for G and G'. At step 0, the contribution of 7 indicates the graphs are composed of very similar building blocks. Both graphs contain roughly the same distribution of labels (mostly one of each number).

At step 1, the contribution of 1 is very low (compared to the theoretical maximum of 6 if the graphs were isomorphic). This indicates that despite having the same nodes, the wiring is different.