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Lab session # 2
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1 Question 1

Let's say we have an undirected graph with n nodes. Each node can connect to n-1 nodes. Therefore, because we have to take into account the duplicates, the maximum number of edges for a graph composed of n nodes is $\frac{n(n-1)}{2}$.
For triangles, if we use combinatorics, then we have $\binom{n}{3} = \frac{n!}{3!(n-3)!}$, the maximum number of triangles in an undirected graph.

2 Question 2

Two isomorphic graphs have the same connectivity (degree distribution) and the same structure. In a more rigorous and mathematical way to say it, as the problem statement recalls, two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic, if there is a bijective mapping $f : V_1ßV_2$ such that $(v_i, v_j) \in E_1$ if and only if $(f(v_1), f(v_2)) \in E_2$.
However, two graphs that have the same degree distribution and the same number of nodes, aren't always isomorphic. Here is a counter-example below :

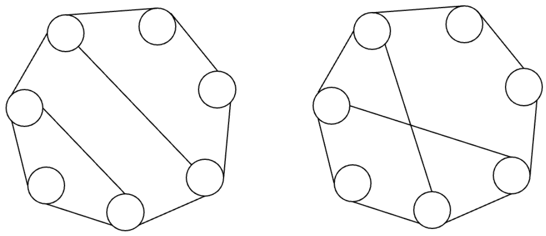

Figure 1: 2 graphs with identical degree distribution but not isomomorphic

3 Question 3

The global clustering coefficient is defined as follows:

$$\text{Global clustering coefficient} = \frac{\text{number of closed triplets}}{\text{total number of triplets}}. \tag{1}$$

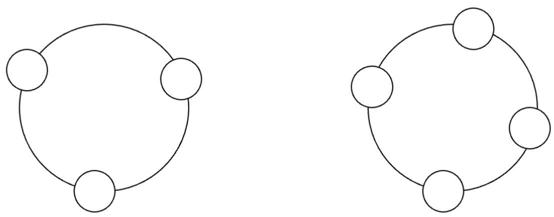

Figure 2: A circle graph on 3 vertices (on the left) and a circle graph on 4 vertices (on the right)

The circle graph of 3 vertices, has only one closed triplet and 0 open triplets. Therefore the global clustering coefficient of the graph with 3 vertices is 1.

However, for the circle graphs of more than 4 vertices, the global clustering coefficient is equal to 0, as they don't have close triplets.

4 Question 4

$$\begin{aligned}
\sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}([u_1]_i - [u_1]_j)^2 &= \sum_{i=1}^{n}\sum_{j=1}^{n}(A_{ij}([u_1]_i))^2 - 2A_{ij}[u_1]_i[u_1]_j + A_{ij}([u_1]_i))^2) && (2)\\
&= \sum_{i=1}^{n}(d_i([u_1]_i))^2 - 2\sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}[u_1]_i[u_1]_j + \sum_{j=1}^{n} d_j([u_1]_i))^2) && (3)\\
&= 2(\sum_{i=1}^{n}(d_i([u_1]_i))^2 - \sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}[u_1]_i[u_1]_j && (4)\\
&= 2(u^T Du - u^T Au) = 2u^T(D-A)u && (5)\\
&= 2u^T D(I - D^{-1}A)u = 2u^T DL_{rw}u && (6)\\
&= 2u^T D\lambda_{smallest} && (7)
\end{aligned}$$

5 Question 5

The computation of the modularity for the first graph (on the left) :

$$Q = \sum^{n_c} \frac{l_c}{m} - (\frac{d_c}{2m})^2 \tag{8}$$

$n_c = 2$
$m = 14$
$d_{orange} = 2 \times 4 + 2 \times 3 = 14$
$l_{orange} = 6$
$d_{blue} = 2 \times 4 + 2 \times 3 = 14$
$l_{blue} = 6$

Therefore,

$$\begin{aligned}
Q_{\text{first graph}} &= \frac{l_{orange}}{m} - (\frac{d_{orange}}{2m})^2 + \frac{l_{blue}}{m} - (\frac{d_{blue}}{2m})^2 && (9)\\
&= 2 \times (\frac{6}{14}) - (\frac{14}{2 \times 14})^2 && (10)\\
&= 0,35714 && (11)
\end{aligned}$$

The computation of the modularity for the second graph (on the right) :
$n_c = 2$
$m = 14$
$d_{orange} = 2 \times 4 + 3 = 11$
$l_{orange} = 2$
$d_{blue} = 2 \times 4 + 3 \times 3 = 17$
$l_{blue} = 5$

Therefore,

$$\begin{aligned}
Q_{\text{second graph}} &= \frac{l_{orange}}{m} - (\frac{d_{orange}}{2m})^2 + \frac{l_{blue}}{m} - (\frac{d_{blue}}{2m})^2 && (12)\\
&= (\frac{2}{14} - (\frac{11}{2 \times 14})^2) + (\frac{5}{14} - (\frac{17}{2 \times 14})^2) && (13)\\
&= -0,0229 && (14)
\end{aligned}$$

6 Question 6

Computation of the kernel of (P_4,P_4) :

P_4 has :

- 3 edges of label 1

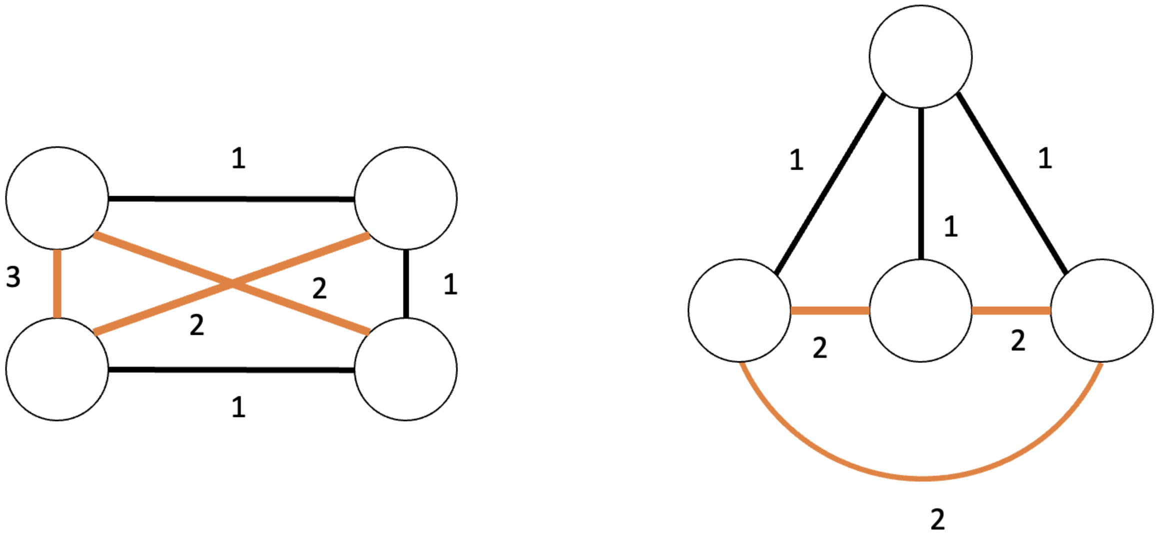

Figure 3: Graphs (P_4 on the left and S_4 on the right) after the Floyd Transformation

- 2 edges of label 2
- 1 edge of label 3

Therefore, $k(P_4, P_4) = 3 \times 3 + 2 \times 2 + 1 \times 1 = 14$

Computation of the kernel of (P_4,S_4) :

P_4 has :

- 3 edges of label 1
- 2 edges of label 2
- 1 edge of label 3

S_4 has :

- 3 edges of label 1
- 3 edges of label 2
- 3 edge of label 3

Therefore, $k(S_4, P_4) = 3 \times 3 + 2 \times 3 + 1 \times 3 = 18$

Computation of the kernel of (S_4,S_4) :

S_4 has :

- 3 edges of label 1
- 3 edges of label 2
- 3 edge of label 3

Therefore, $k(S_4, P_4) = 3 \times 3 + 3 \times 3 + 3 \times 3 = 27$

7 Question 7

In the example below (figure 4), the graphlet kernel is equal to 0. In fact, the graph on the left has $f_G = (4, 0, 0, 1)$ and the graph on the right has $f_{G'} = (0, 4, 0, 0)$. Therefore, the graphlet kernel is equal to $k(f_G, f_{G'}) = f_g^T f_{G'} = 0$.
On figure 5, the graphlet kernel is equal to 0 too. In fact, the graph on the left has $f_G = (8, 0, 0, 0)$ and the graph on the right has $f_{G'} = (0, 6, 12, 0)$. Therefore, the graphlet kernel is equal to $k(f_G, f_{G'}) = f_g^T f_{G'} = 0$.
The fact that the kernel of 2 graphs is equal to 0 means that the vectors that capture the features of the graphs are orthogonal.

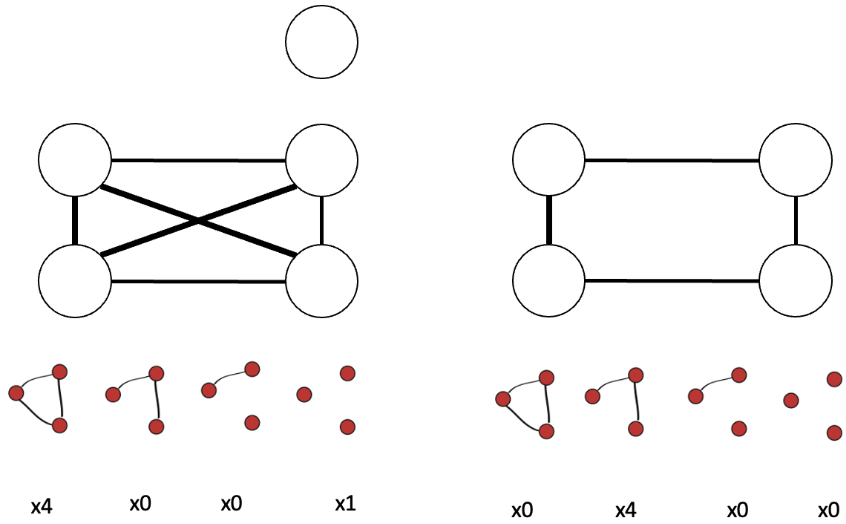

Figure 4: Example of 2 graphs and their graphlets, where the graphlet kernel is equal to 0

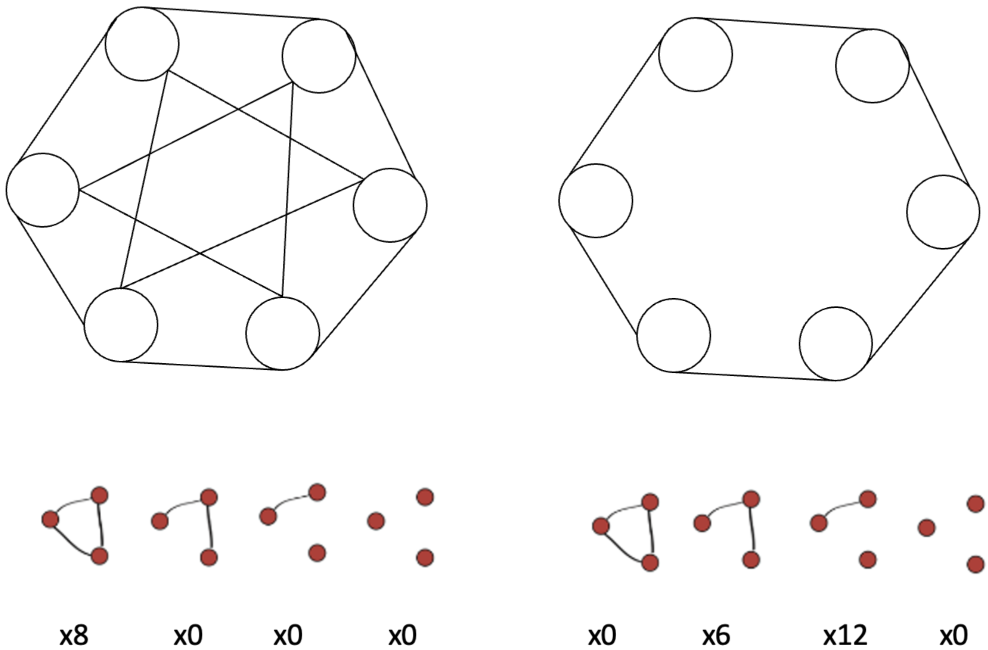

Figure 5: Example of 2 graphs and their graphlets, where the graphlet kernel is equal to 0