BENYAMINA Elyas
elyas.benyamina@ens-paris-saclay.fr

Lab session # 2
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1 Question 1

The maximum number of edges of an undirected graph of n nodes without self-loops is reached when all the nodes are connected, and in this case there are $\frac{n(n-1)}{2}$ edges (node 1 is connected to $n-1$ nodes, then node 2 is connected to $n-2$ other nodes,...., and node 2 is connected to 1 other node, and by summing we get $\sum_{k=1}^{n-1} = \frac{n(n-1)}{2}$).

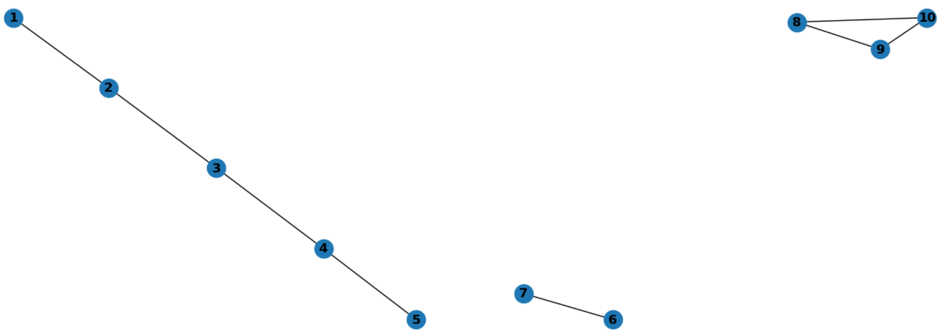
The maximum number of triangles of an undirected graph of n nodes without self-loops is still reached when all the nodes are connected, and in this case there are $\binom{n}{3}$ triangles, because we are looking for how many possibilities there are to take 3 nodes (to link them).

To sum up,

1. Maximum number of edges: $\sum_{k=1}^{n-1} = \frac{n(n-1)}{2}$
2. Maximum number of nodes: $\binom{n}{3}$

2 Question 2

If two graphs have identical degree distributions, they are not isomorphic to each other in general.
Here is a counterexample for graphs with 5 nodes. We can prove it with absurd.



(a) (b)

Figure 1: Graphs which share same degree distribution but are not isomorphic (first graph is composed of nodes 1, 2, 3, 4 and 5, second graph is composed of nodes 6, 7, 8, 9 and 10)

Suppose that they are isomorphic and we consider f the bijective mapping from graph 1 to graph 2.

- **If** $f(1) = 6$ **(same proof if** $f(1) = 9$ **or** $f(1) = 10$**)**, then $f(2) = 7$ (because the only possibility to have an edge between $f(1)$ and $f(2)$ is to have $f(2) = 7$.
  But, we have an edge between $f(2)$ and $f(3)$ so, $f(3) = 6$, which is absurd because f would not be bijective.
- **If** $f(1) = 8$ **(same proof if** $f(1) = 9$ **or** $f(1) = 10$**)**, then $f(2) = 9$ or $f(2) = 10$.
  If $f(2) = 9$, then $f(3) = 10$, but because f is bijective, $f(4)$ has to be 6 or 7.
  So, there is no edge between $f(4)$ and $f(3)$ but there is an edge between 4 and 3, which is absurd. Same applies if $f(2) = 10$.

We can conclude that there is no f function that suits, and so graph 1 and 2 are not isomorphic.

Note that we can prove that if two graphs have a number of nodes less or equal to 4, they are isomorphic if and only if they share same degree distribution.

3 Question 3

For $n \geq 3$, the cycle graph on v verticles C_n has n open triplets and no closed triplet (because each node is connected to two nodes only, and these two nodes are not connected).
Then, global clustering coefficient is $\frac{0}{n+0} = 0$.

4 Question 4

Let $\mathbf{u}_1 \in \mathbb{R}^n$ denote the eigenvector associated with the smallest eigenvalue (we nothe this eigenvalue λ) of $\mathbf{L_{rw}}$ and let $[\mathbf{u}_1]_i$ denote the i-th element of $\mathbf{u}_1$.
We have

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\mathbf{A}_{ij}\left([\mathbf{u}_1]_i - [\mathbf{u}_1]_j\right)^2 = \sum_{i=1}^{n}\sum_{j=1}^{n}\mathbf{A}_{ij}\left([\mathbf{u}_1]_i\right)^2 + \sum_{i=1}^{n}\sum_{j=1}^{n}\mathbf{A}_{ij}\left([\mathbf{u}_1]_j\right)^2 - 2\sum_{i=1}^{n}\sum_{j=1}^{n}\mathbf{A}_{ij}\left([\mathbf{u}_1]_i \cdot [\mathbf{u}_1]_j\right)$$

As, A is the adjency matrix (and it is symmetric because we are working with undirected graphs) of the graph and D the diagonal degree matrix of the graph, we have $\sum_{j=1}^{n}\mathbf{A}_{ij} = D_{ii}$. So, we can write :

$$\begin{aligned}
\sum_{i=1}^{n}\sum_{j=1}^{n}\mathbf{A}_{ij}\left([\mathbf{u}_1]_i - [\mathbf{u}_1]_j\right)^2 &= \sum_{i=1}^{n} D_{ii}\,[\mathbf{u}_1]_i^2 + \sum_{j=1}^{n} D_{jj}\,[\mathbf{u}_1]_j^2 - 2\sum_{i=1}^{n}\sum_{j=1}^{n}\mathbf{A}_{ij}\left([\mathbf{u}_1]_i \cdot [\mathbf{u}_1]_j\right) \\
&= 2\sum_{i=1}^{n} D_{ii}\,[\mathbf{u}_1]_i^2 - 2\sum_{i=1}^{n}\sum_{j=1}^{n}\mathbf{A}_{ij}\,[\mathbf{u}_1]_i \cdot [\mathbf{u}_1]_j \\
&= 2\sum_{i=1}^{n}[\mathbf{u}_1]_i\, 2\sum_{k=1}^{n} D_{ik}\,[\mathbf{u}_1]_k - 2\sum_{i=1}^{n}\sum_{j=1}^{n}[\mathbf{u}_1]_i\,\mathbf{A}_{ij}\,[\mathbf{u}_1]_j \\
&= 2\sum_{i=1}^{n}[\mathbf{u}_1]_i\,(D\,[\mathbf{u}_1])_i - 2\sum_{i=1}^{n}\sum_{j=1}^{n}[\mathbf{u}_1]_i\,\mathbf{A}_{ij}\,[\mathbf{u}_1]_j \\
&= 2^t\,[\mathbf{u}_1]\,D\,[\mathbf{u}_1] - 2^t\,[\mathbf{u}_1]\,A\,[\mathbf{u}_1] \\
&= 2^t\,[\mathbf{u}_1]\,(D-A)\,[\mathbf{u}_1] \\
&= 2^t\,[\mathbf{u}_1]\,DL\,[\mathbf{u}_1] \\
&= 2\lambda^t\,[\mathbf{u}_1]\,D\,[\mathbf{u}_1] \\
&= 2\lambda\sum_{i=1}^{n} D_{ii}\,[\mathbf{u}_1]_i^2
\end{aligned}$$

5 Question 5

For the first graph, we have

$$\begin{aligned}
n_c &= 2 \\
m &= 14 \\
l_1 &= 6 \\
l_2 &= 6 \\
d_1 &= 14 \\
d_2 &= 14
\end{aligned}$$

So, we can compute and we get the modularity,

$$Q = \frac{5}{14} \approx 0.36$$

.

For the second graph, we have

$$
\begin{aligned}
n_c &= 2 \\
m &= 14 \\
l_1 &= 2 \\
l_2 &= 5 \\
d_1 &= 11 \\
d_2 &= 17
\end{aligned}
$$

So, we can compute and we get the modularity,

$$Q = -\frac{9}{392} \approx -0.023$$

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6 Question 6

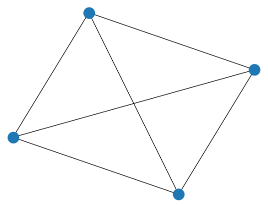
We have $\Phi(P_4) = [3,2,1,0]$, and $\Phi(S_4) = [3,3,0,0]$. So we can compute shortest path kernel for :

1. shortest path kernel of $(P_4, P_4) = 6$
2. shortest path kernel of $(P_4, S_4) = 5$
3. shortest path kernel of $(S_4, S_4) = 6$

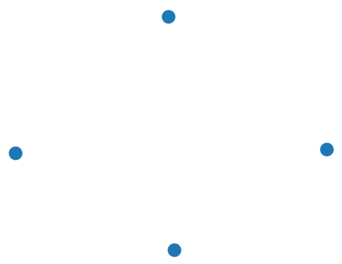
7 Question 7

Let k denote the graphlet kernel that decomposes graphs into graphlets of size 3.
Let also G, G' denote two graphs and suppose that $k\left(G, G'\right) = f_G^\top f_{G'} = 0$.
It implies that for all $i \in \{1,2,3,4\}$, $(f_G)_i = 0$ or $(f'_G)_i = 0$.
By definition of f_G and f'_G, it implies that if we take a subgraph of size 3 of G and G', they cannot be isomorphic.
Here is an example with G and G' which have four nodes (we can take three nodes for simple example as there is only one subgraph or even less, because there is no subgraph of size three).

Let's take G the graph of four nodes with all nodes connected and G', the graph of four nodes with no edges.



(a)



(b)

Figure 2: Graphs G and G'

We have subgraphs of size 3 of G who are isomorphic to G_1 and subgraphs of size 3 of G' who are isomorphic to G_4.

So, $f_G = \begin{pmatrix} 4 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ and, $f_{G'} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 4 \end{pmatrix}$, and we have $k\left(G, G'\right) = f_G^\top f_{G'} = 0$.