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Lab session # 5
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1 Questions :

1.1 Question 1:

The max number of edges corresponds to the case where each node will be connected to the n-1 other nodes. $N_{max} = (n-1) + (n-2) + \ldots + 2 + 1 = \sum_{k=1}^{n-1} k = \frac{n(n-1)}{2}$

The max number of triangles is the number of combinations of $\binom{n}{3}$

1.2 Question 2:

There are a lot of edges that have low degrees and very few that have very high degrees. Which can asses the amount and quantity of hubs (influencers) present in that graph. This is called a power law distribution

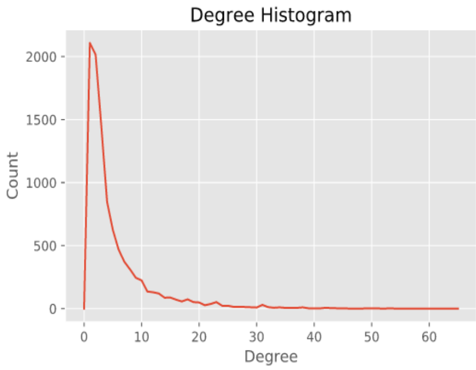

Figure 1: The histogram of nodes degrees

1.3 Question 3:

The goal is to force the coordinates of nodes that have a large similarity to be close together. Let f_i be the representation of the node i Then we need to minimize

$$f^T L f = \sum_{ij} w_{ij} (f_i - f_j)^2$$

Since L is a symetric matrix positive semi-definite, we can apply a spectral decomposition on it and L has N all non negative real eigenvalues. Since $1^T L 1 = 0$, (0,1) is a trivial eigenpair, we look at the next non trivial eigenvalues. Let us consider $L = U^T D U$ the eigen decomposition of L We have

$$f^T L f = f^T U^T D U f = (Uf)^T D (Uf)$$

If we denote the vector $\alpha = Uf$ we have that :

$$f^T L f = \alpha^T D \alpha = \sum_i^N \lambda_i \alpha_i^2$$

And thus the eigenvectors corresponding to the smallest eigenvalues are the one that minimize $f^T L f$

1.4 Question 4:

$$m = 10$$

$$l_{green} = 1$$

$$l_{gray} = 5$$
$$l_{blue} = 3$$

$$d_{green} = 2$$

,

$$d_{gray} = 2 + 3 + 3 + 3 = 11$$

,

$$d_{blue} = 2 + 2 + 3 = 7$$

$Q = 1/10 - (2/20)^2 + 5/10 - (11/20)^2 + 3/10 - (7/20)^2 = 0.464$

1.5 Question 5:

An example of two non-isomorphic graphs which are mapped to the same representation by the shortest path kernel is:

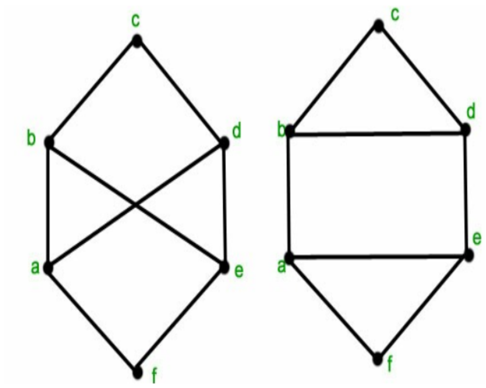

Figure 2: Exemple of Non-isomorphic graphs with same SP kernel

It's clear that the graphs are non-isomorphic but the SP kernal is equal to $\phi = [8, 6, 1]$ for both of them.

1.6 Question 6:

We observe that the shortest path kernel achieves a very high accuracy whereas the graphlet kernel has a very bad performance.

The high accuracy of the SP-kernel is explained by the fact that the cyclic graphs do not have high shortest path distances. Thus when performing the dot product of the SP-kernel of such a graph with a path graph (given a path graph G of n nodes, its SP-kernel is $\phi_{sp}(G) = [(n-1), (n-2), ..., 1]$) the sum is not very big as it is the case when performing the dot product with another path graph. So it is much easy to classify using these "features" (that correspond to the similarity of the graph with all the graphs in the training set) because they are directly correlated to the graph structure.

The poor accuracy of the graphlet kernel is that, when sampling 3 nodes in the graph randomly, there is no distinction between a path graph or a cyclic graph. Indeed they can both have any of the structures of the graphlets (1, 2, 3 or 4) and thus this kernel is not very adequate for this kind of task.f

References