BT5420 - COMPUTATIONAL SYSTEMS BIOLOGY

Assignment 2

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Question 1

http://networkrepository.com/ENZYMES8.php - This is a Labelled network of enzymes.

The network does not have edge weights. It is an undirected graph.

Assortativity -

This was computed based on two methods, both of which are reported.

The <u>first method</u> is based on the formula given in Textbook (NewMan formula) where the nodes of the network was classified into two categories – high degree and low degree. The threshold was set to be the average degree of the network. A 2*2 matrix was constructed based on the number of interactions between the two types of nodes (This will yield a symmetric matrix).

$$r = \frac{Tr \ e - \|e^2\|}{1 - \|e^2\|}$$

The assortativity coefficient calculated by this method was found to be 1.3822.

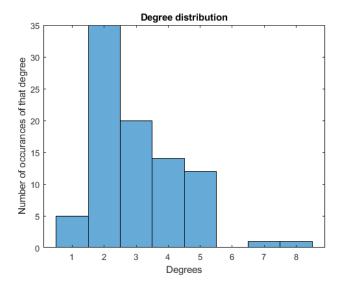
The <u>second method</u> was to get a simple Pearson Correlation coefficient between the left_index_degrees and right_index_degrees of all edges. This was computed as follows:

This will yield a 2*2 matrix with diagonal elements as 1.0 always. The off-diagonal element specifies the R value which is the correlation coefficient between the two vectors.

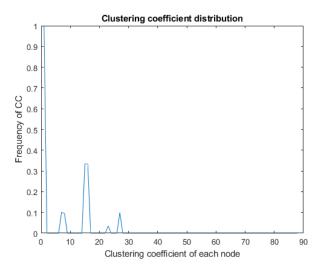
The assortativity coefficient calculated by this method was found to be 0.0685.

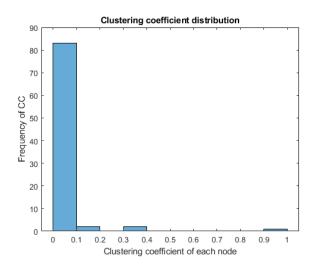
Inference - Therefore, we can conclude that the degrees of the network are very minimally positively correlated/assorted.

Degree Distribution



Distribution of Clustering Coefficient -





(d)

- The network appears to have a degree distribution that follows Power Law.
- The trend of the distribution of Clustering coefficient decreases as the node degree increases. This distribution also follows a power law. This implies that the low-degree nodes belong to very dense sub-graphs and those sub-graphs are connected to each other through hubs.

Both the above characteristics hint towards the same fact that the network resembles a <u>scale-free</u> <u>network.</u>

Question 2

Network A was constructed as a <u>regular lattice</u> with number of nodes = 100 and each node was connected to 3 nodes on the right and 3 to its left (There is no directionality involved. Left and right were mentioned to understand the architecture of the network.)

Rewiring a network -

Network A was rewired in the following way.

I did an iteration through all edges. While we are under the specified probability, I generate a random number. I check if the random number is not the same as neighbours of the left_index of a particular edge, or the left_index itself. In that case, I cut the already existing edge and create a new one between (left index, the generated random number). (Cut and create was done by just changing the right_index of the edge). At the end f every iteration, I updated the network with the changes in edge list (eA as in the program), so that in each round, neighbour vector is found appropriately.

The program is written as follows:

```
function [B] = hw2 2 rewiring(A,p)
```

where A is the network itself (a Graph variable) and p is the probability of rewiring an edge. The function returns B, which is an adjacency matrix of the newly formed/rewired network.

As the rewiring function is called within the main program of 2^{nd} question, the probability of rewiring (p) was input as an argument to this function while calling.

The program is written as follows:

```
function [] = hw2 2(p)
```

Final values – (for input parameter p = 0.2)

Diameter – This is the length of the longest geodesic (longest shortest path!) in the graph.

Network
$$A = 17$$

Network B = 6

Characteristic path length – This measures the average separation between two nodes in a network.

Network
$$A = 8.7576$$

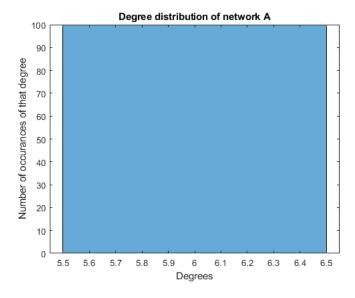
Network
$$B = 3.2133$$

Global clustering coefficient – C can be thought to measure the cliquishness of a node's neighbourhood. The mean clustering coefficient (CC) of the network is its global CC as well.

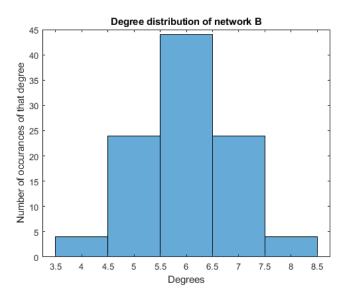
Network
$$A = 0.6000$$

Network
$$B = 0.3385$$

Degree distribution of Network A -



Degree distribution of Network B -



Network A and B are as follows -

