Assignment 3

BT5240 Computational Systems Biology | Jan - May 2022
Network Centrality and Flux Balance Analysis
March 29, 2022

Due Date: 8th April, 2022
Maximum marks: 25

Academic Integrity: You are allowed to discuss the problems verbally with your friends, but copying or looking at codes (either from your friend or the Web) is not permitted. Transgressions are easy to find, and will be reported to the "Sub-committee for the Discipline and Welfare of Students" and will be dealt with very strictly. Mention any collaboration (discussions only!) in your solutions.

Submission: Since this is a computational assignment, we would also like to look at your codes. Submit your assignment as one zip file by uploading it at http://tinyurl.com/bt5240-submit
Your zip file should be named something like BTyyBxxx.zip, based on your roll number. This zip file must contain a single neatly typeset PDF of your solutions (named BTyyBxxx.pdf) including well annotated the plots and figures of legible fontsize as well as the codes used for each of problems in a separate folder codes with proper annotations.

Problem 1: Network Centrality for Transcriptional Regulatory Network (12 marks)

a) Use the *E. coli* transcription network given here and convert it into a network in MATLAB. Ignore the sign of the edges. (2 marks)

   [Note: Node information is given here. Additional information and description of the network can be found here.]

b) Calculate the following quantities for each node in the network and report the top five transcription factors according to each of these centrality measures. (7 marks)
   i) Degree Centrality
   ii) Closeness Centrality
   iii) Shortest Path Betweeness Centrality
   iv) Radiality
   v) Integration

   [Hint: $D = (dist(i,j))$
   Reverse Distance Matrix RD, $RD_{ij} = diameter(G) + 1 - D_{ij}$ where diameter(G) is the diameter of the Graph G.

Radiality is defined as $C_{rad}(i) = (\sum_{i \neq j} RD_{ij}) / (n - 1)$ and Integration is defined as

$C_{int}(j) = (\sum_{i \neq j} RD_{ij}) / (n - 1)]$

c) Calculate the kendall correlation coefficient among all these measures and report a 5 x 5 table such that the (i,j) entry signifies the kendall correlation coefficient between i^{th} centrality and j^{th} centrality measure. (3 marks)

Problem 2: Starting with Flux Balance Analysis (13 marks)

a) Download the model of the Staphylococcus aureus subsp. aureus N315 - iSB619 from here and report the maximum growth rate in the given conditions (8 marks)
   i) With glucose (100 $mmolgDW^{-1}h^{-1}$) as a substrate under aerobic condition
   ii) With glucose (100 $mmolgDW^{-1}h^{-1}$) as a substrate under anaerobic condition
   iii) With D-ribose (100 $mmolgDW^{-1}h^{-1}$) as a substrate under aerobic condition
   iv) With Fructose (100 $mmolgDW^{-1}h^{-1}$) as a substrate under aerobic condition

b) Analyze the lethal genes observed under the different carbon sources and comment on the results. (5 marks)