EE430

Introduction to Systems Biology

Spring 2021 Final

Due 16.6.2021, midnight

Instructions:

This is a take-home test. You are asked to answer the test on your own and return the answers in a single PDF document with your name and student identification number in the file name. Sharing of ideas and verbal discussions on the test questions are encouraged but sharing of results and/or text is not. Your name on your test acts as a statement on your part that you have fully complied with the student honor system. Make sure that you show your work and justify your answers. Correct answers to wrong questions are not creditable.

Question 1 (50 points) Consider the following system of equations that govern the enzyme-mediated chemical reaction between X and Y:

1) $X + Y \rightarrow XY$

2) $XY \rightarrow X + Y$

3) $X + E \rightarrow XE$

4) $XE \rightarrow X + E$

5) $Y + E \rightarrow YE$

6) $YE \rightarrow Y + E$

7) $XE + Y \rightarrow XY + E$

8) $YE + X \rightarrow XY + E$

with the corresponding reaction rate constants $k_1, k_2, \ldots, k_8$ set arbitrarily in such a way that XY forms in the presence of the enzyme E and very little otherwise.

a) (10 points) Write down the ordinary differential equations of the dynamic model that governs the rate of change in time of all reactant concentrations in this system.

(Note: Assume that the minimal integer powers of the reactant concentrations in the reaction rate expressions match their respective coefficients in the biochemical reactions.)

b) (20 points) Numerically solve this system until steady state and plot the transient behavior of all reactants for time $t > 0$ along with the moiety groups subject to the initial conditions $[\mathrm{X}]|_{t=0} = [\mathrm{Y}]|_{t=0} = 1$ and $[\mathrm{E}]|_{t=0} = [\mathrm{XE}]|_{t=0} = [\mathrm{YE}]|_{t=0} = [\mathrm{XY}]|_{t=0} = 0$, i.e. in the absence of the enzyme E.

c) (20 points) Numerically solve this system until steady state and plot the transient behavior of all reactants for time $t > 0$ along with the moiety groups subject to the initial conditions $[\mathrm{X}]|_{t=0} = [\mathrm{Y}]|_{t=0} = [\mathrm{E}]|_{t=0} = 1$ and $[\mathrm{XE}]|_{t=0} = [\mathrm{YE}]|_{t=0} = [\mathrm{XY}]|_{t=0} = 0$, i.e. in the presence of the enzyme E. Show that the steady state concentration of XY is much larger in the presence of the enzyme E.

Question 2 (50 points) Consider an undirected network with the following degree distribution.

- 6 nodes of degree 1
- 4 nodes of degree 2
- 3 nodes of degree 3
- 1 node of degree 5

a) (10 points) Draw a network graph satisfying the degree distribution given above.

(Note: The connectivity of a graph is fully determined by its adjacency matrix. Computer algorithms can be used to generate many adjacency matrices and determine if they fit a desired selection criterion.)

b) (30 points) Enumerate the nodes in your graph and calculate their degrees as well as clustering coefficients.

c) (10 points) Calculate the eigenvector centrality of your graph and rank the nodes in a decreasing order of centrality.