AMATH 422 HW 1 Due 10/2/2024

I Project warmup: (This is Ellner and Guckenheimer Exercise 1.1:). Turn this writeup in as a markdown cell within an ipython notebook! See the markdown cheatsheet linked from our python tutorial for guidance, and remember that equations can be formatted using dollar signs (LaTex). Find a scientific research paper published that uses a dynamic model in a biology area of interest to you, read the paper, and turn in a short writeup with one-paragraph answers to the following questions.

(a) Give the complete citation for the paper: authors, date, journal, pages.
Ma W, Trusina A, El-Samad H, Lim WA, Tang C. Defining network topologies that can achieve biochemical adaptation. Cell. 2009 Aug 21;138(4):760-73. doi: 10.1016/j.cell.2009.06.013. PMID: 19703401; PMCID: PMC3068210.

(b) What was the purpose of the model { that is, what was accomplished by building and using the model?
The purpose of the model in the paper is to find specific characteristics of adaptive signaling systems. Adaptive signaling systems can reset themselves after responding to a stimulus. Adaption is important in signaling networks to expand the input range, detect changes in input and maintain homeostasis in the presence of changes in input. The model used was three-node enzyme processes with one node that receives input, a second node that transmits output, and a third node that can play diverse regulatory roles. With three nodes there are 19,683 total topologies, but only 16,038 are usable, because they have direct links from input to output. Each topology had 10,000 parameter sets sampled uniformly and evaluated for their sensitivity to input change and adaption precision. The overall performance of topology was measured by robustness. The model used Michaelis-Menten ordinary differential equations to model enzyme kinematics. The main finding of the paper was that their model showed only a finite set of solutions for robustly achieving adaptation in signaling pathways.

(c) What are the parameters (fixed constants that the modeler chooses) of the model? What are the variables that change over time and/or change as a result of these parameters (sometimes called state variables)?
The parameters in the paper were specifically varied, because certain topologies may be more favorable due to specific parameter constraints. There are a total of 16,038 possible three-node topologies that have a causal link from the input node to the output node. Using the Latin hypercube sampling method, each node was sampled by 10,000 sets of network parameters, and then by characterized the resulting behavior of the ability of the circuit to adapt. The precise implementation of the node topology could differ dramatically due to the parameters influenced by the biochemical details and evolutionary history. The model used

ordinary differential equation to model the reactions, Michaelis Menten equations, with dissociation constant Km and catalytic rate constants Kcat.

(d) Identify one of the models simplifying assumptions { some known aspect of the real world that the model omits or simplifies.

The model's simplifying assumptions are the Michaelis Menten Steady State Equilibrium and Noncooperative binding. Noncooperative Binding is when the binding of one molecule to the enzyme does not alter the affinity of the molecule to the enzyme. Michaelis Menten Steady State Equilibrium is a common and reasonable simplification of enzyme catalyzation of reaction based on specific criteria. The paper states that the assumptions do no not significantly alter the results, when using the mass actions rate equation of Michaelis-Menten or when using nodes of higher cooperativity.

II Additional Turn this in as markdown and/or code cell(s) within the same ipython notebook!. Write down at least two additional brief python or notebook tips / tricks, or GOTCHAs { beyond what is in the tutorial { to share with the class.

Tip and Trick number one:

Organizing files should be consistent across classes and subjects. Having to find a file but not understanding where it is will only grow the problem.

Tip and Trick number two:

Just because you understand your code now in this moment does not mean you understand your code in a week or a day or even in an hour. Having clear commenting and straightforward can save a lot of time in the future. Especially forgetting syntax.

Tip and Trick number three:

matlab code starts arrays with 1. Python code starts arrays with 0. Big difference.

In [ ]: