Each homework consists of 3 problems, and you are expected to spend 30 min to 1 hour on each problem, but definitely less than 1 hour. If you find yourself spending more than 1 hour, you are probably overthinking about it. Problems with (*) are for further explorations which may take longer, and are OPTIONAL if you are short on time.

1 Analysis of dynamics by phase portrait

For this problem, we consider a series of classic dynamical systems and use the techniques we learned in class to understand their dynamics.

1.1 Downward pendulum

Consider a pendulum suspending from a point, with θ denoting it makes with the vertically downward axis (e.g. on the left), so $\theta = \pi$ is vertically upward, for example. Let m denote the mass of the point mass at the end of the pendulum, and assume the rod of the pendulum is mass-less. Let L denote the length of the pendulum.

1. Show that the dynamics of the system is
$$g \sin\theta = -L\ddot{\theta}. \tag{1}$$

2. Transform this into a state system, by defining the state variables $x_1 = \theta$ and $x_2 = \dot{\theta}$. Show that the system is
$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_2 \\ -\frac{g}{L}\sin x_1 \end{bmatrix}. \tag{2}$$

3. Draw the phase portrait of the system. Note that x_1 can go beyond $-\pi$ to π, since the pendulum and rotate several rounds. A good choice for the range of x_1 axis can be $[-3\pi, \pi]$. (Hint: What does energy conservation imply for the phase portrait?)

   Describe the different types of dynamic trajectories this system can have.

4. Do the small-angle approximation to linearize the system. In other words, linearize around the fixed point $\theta = \dot{\theta} = 0$, i.e. $x_1 = x_2 = 0$. How does the linearized system compare with the spring system we looked at in class? What does this imply about its dynamics? Compare the dynamics of the linearized system with the dynamics of the full system analyzed via phase portrait above, what are captured by the linearization and what are not captured?

1.2 Upward or inverted pendulum (*)

Now we consider the upward pendulum, or the inverted pendulum. This is often considered the first example in control systems.

Let φ denote the angle the pendulum makes relative to the vertically upward position, so $\varphi = \pi - \theta$ if the angle φ makes is on the same side (e.g. left) of the vertical axis as the angle made by θ, where θ is the angle of the downward pendulum in the previous problem.

1. Show the dynamics for the inverted pendulum is
$$g \sin\varphi = L\ddot{\varphi} \tag{3}$$

   and the state system dynamics is
$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_2 \\ \frac{g}{L}\sin x_1 \end{bmatrix}, \tag{4}$$

where $x_1 = \varphi$, $x_2 = \dot{\varphi}$.

Is the fixed point $x_1 = x_2 = 0$ locally stable? What is the linearized system?

2. We can add control to stabilize the system around the fixed point. In other words, we can add control to balance the inverted pendulum at its upward position. What control can achieve this objective?

   We can first try a passive control by adding friction. Add a friction term to the linearized system and analyze the local stability of the fixed point. Is it enough to stabilize the upward position?

3. Let us try adding a more active control. Imagine a hand or a cart supporting the inverted pendulum at the bottom, and exerting a horizontal force F. This is called an inverted pendulum on a cart.

   Let x denote the horizontal location of the bottom of the inverted pendulum, with positive x pointing to the opposite side of the vertical axis as angle φ (e.g. positive x is on the right.) Then its acceleration $\ddot{x}$ captures the result of the force F. The resulting equations of motion is

   $$g \sin \varphi + \ddot{x} \cos \varphi = L\ddot{\varphi}. \tag{5}$$

   Write this as a control system, with state variables $x_1 = \varphi$, $x_2 = \dot{\varphi}$, and $u = \ddot{x}$, we have

   $$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_2 \\ \frac{g}{L}\sin x_1 \end{bmatrix} + \begin{bmatrix} 0 \\ u \cos x_1 \end{bmatrix}. \tag{6}$$

   Linearize the system around the operating point $x_1 = x_2 = u = 0$ (operating point is like a fixed point but for a control system, so the control variable is also fixed.) Write the system in the form of $\frac{d}{dt}x = Ax + Bu$, where A and B are constant matrices.

4. Intuitively, to stabilize the inverted pendulum by the horizontal force at the bottom, when φ tilts towards the left, we also need to accelerate to the left. This means, for positive $\varphi = x_1$, we want a negative $\ddot{x} = u$. If we give them a linear relation, we obtain $u = -k_s x_1$, where k_s is the linear coefficient. This is like adding a spring on the pendulum point mass as the controller. What's the resulting closed loop dynamics of the linearized system? (Open loop refers to the case $u = 0$, and closed loop refers to when the controller u with its dependence on x is added.) Can the upward position be stabilized under this controller, maybe for some parameters? How does the closed loop dynamics compared with the downward pendulum? What would you add to the controller to further stabilize the system?

   Food for thought: we analyzed and designed the control of the inverted pendulum by linearization around the upward position, and the resulting behavior with the controller added is indeed that we stabilized the system at the upward position. But we are told that linearization only holds for the local behavior around a fixed point of a nonlinear system! Does our analysis for the stabilization controller based on the linearized model holds true when the controller is added to the full nonlinear system, assuming we start with an initial condition that is close to the fixed point? Why or why not?

2 Analog computation by chemical reaction networks

We know that chemical reaction networks (CRNs) with mass action kinetics, i.e. elementary reactions, have monomial rates. For example, elementary reaction $\alpha_1 X_1 + \cdots + \alpha_n X_n \xrightarrow{k} \cdots$ has reaction rate $k x_1^{\alpha_1} \ldots x_n^{\alpha_n}$, where x_i denotes the concentration of chemical species X_i. This means most systems with polynomial dynamics can be implemented by CRNs. Therefore, if any sort of computational problem can be solved by polynomial dynamics, then we can write down a set of chemical reactions that performs the analog computation to solve this problem.

2.1 Square root

Let us consider the problem of computing the square root of a quantity X. Let us assume this input quantity is given to us as the concentration of a chemical species. We need to come up with a CRN such that the concentration of another chemical species Y is the output that performs the square root computation. In other words, at steady state, $y = \sqrt{x}$, where x and y are concentrations of X and Y species.

1. Consider the reactions $X \xrightarrow{1} X + Z$ and $Z \xrightarrow{1} \emptyset$, what is the rate equation of this CRN, and how is the steady state concentration of z related to x?

2. Construct a CRN involving only X and Y such that $y = \sqrt{x}$ at steady state.

2.2 Decision making in winner take all

(Adapted from course Bio/CS 191 at Caltech taught by Erik Winfree in Winter 2017.)

While it might be obvious that algebraic problems such as taking square roots can be implemented by polynomial dynamical systems, and therefore by CRNs, it is actually the case that polynomial dynamical systems, and CRNs, are Turing universal, i.e. they can perform any computations that a Turing machine can. Therefore, CRNs can actually solve all kinds of complex problems.

Here, we look at one simple case of decision making in winner take all. Imagine we are given two inputs X and Y, and we would like to compare them and let the larger of the two be the winner. We could encode the inputs as initial concentrations of the two chemical species, x_0 and y_0. We could then indicate the winner by letting the winner species take all the concentration, i.e. $(x_\infty, y_\infty) = (x_0 + y_0, 0)$ if $x_0 > y_0$, and $(x_\infty, y_\infty) = (0, x_0 + y_0)$, where x_∞ and y_∞ are steady state concentrations of X and Y, respectively.

1. Consider the following chemical reaction network.

$$\begin{aligned} X + Y &\xrightarrow{1} 2Z, \\ Z + X &\xrightarrow{1} 2X, \\ Z + Y &\xrightarrow{1} 2Y. \end{aligned} \tag{7}$$

   Intuitively describe, if we start with initial condition $(x, y, z) = (x_0, y_0, 0)$, how would the system evolve and what would be the final state of the system? What quantity is conserved?

2. Write down the rate equation for this CRN. How many fixed points does this system have? Which ones are locally stable?

3. Use the conserved quantity to eliminate the z variable, so as to write the system dynamics in terms of just x and y and have an equivalent 2d system. Now draw the phase portrait of the system and analyze its global dynamics. Argue that the dynamics of this system indeed computes winner take all.

4. (Optional) Write computer code using your favorite language to simulate this system, plot time trajectories, and find that the dynamics is indeed as desired. (Hint: This webpage has tutorials and examples on simulating chemical reaction networks using python: `https://biocircuits.github.io/technical_appendices/02b_numerical_odes.html`, and this webpage has similar things using julia: `https://docs.sciml.ai/Catalyst/stable/#doc_index_example`.)

3 Lotka-Volterra

A famous model in biological systems with oscillatory dynamics is the Lotka-Volterra model, or the predator-prey model. It was originally proposed in the 1910s and 1920s to describe oscillatory dynamics seen in chemical reactions and populations of predator and prey fishes in the ocean. Since then, it has been greatly extended and has been developed as the workhorse model for interacting populations and communities in ecology, evolution, and microbiology. Here we use the tools we've learned to look into the oscillatory dynamics of the classic model.

1. The classic Lotka-Volterra model is the following:

$$\begin{aligned} \frac{d}{dt}x &= \alpha x - \beta xy, \\ \frac{d}{dt}y &= -\gamma y + \delta xy. \end{aligned} \tag{8}$$

   Here x is the population of the prey, and y is that of the predator.

   (Food for thought: Could you a chemical reaction network with elementary reactions such that its dynamics is the Lotka-Volterra system?)

   Briefly describe what each term in the model means.

2. Look at the dynamics of the prey if there is no predator, i.e. when y is fixed at $y = 0$. This is a one-dimensional system. What is the behavior and what is the solution?

   This is called the exponential growth model, which captures a rapidly growing population.

3. Look at the dynamics of the predator when the prey is overabundant (i.e. assumed to be held constant at a rather large number.) This is a one-dimensional system. Draw its phase portrait, and describe its dynamics.

   This is called the logistic growth model, which captures a growing population with a saturating carrying capacity determined by the environment.

4. Now look at the full Lotka-Volterra model.

   What are the fixed points of the system? Are they locally stable? Show that $V(x, y) = \delta x - \gamma \log x + \beta y - \alpha \log y$ is a conserved, and notice that it is non-negative since the entropy function $x - a \log x$ is non-negative for $x > 0$ and $a > 0$. (This V is like the energy function for mechanical systems we have studied. Such generalized energy functions that are nonnegative and conserved or decreases over time are called Lyapunov functions, and they can be used to analyze or even design global dynamics.) Draw the phase portrait for the system, and described its dynamics.

5. (Optional) Does the Lotka-Volterra model have a stable limit cycle? If not, then the periodic oscillations observed in the Lotka-Volterra model is rather unsatisfactory. This is because upon slight perturbations of the model's initial conditions, we would have different periods and different amplitudes of oscillations, which makes it seems like the model's periodic behavior is rather fragile. Realistically, the oscillatory behavior must be stable at least to perturbations of relatively small magnitude for us to observe. To fix this problem, let us consider what modifications of the Lotka-Volterra model may make it more realistic such that the periodic behavior has a stable limit cycle.

   This turns out to be a rather non-trivial problem, and took the joint work of quite a few researchers in the field of nonlinear dynamical systems from 1960s to 1980s to fully understand. For example, it is known that for all generalized Lotka-Volterra models $\frac{d}{dt}x_i = b_i x_i + \sum_{j=1}^{n} a_{ij} x_j$ for $i = 1, \ldots, n$, as long as it is in two dimensions, i.e. $n = 2$, there are no stable limit cycles. However, there exists stable limit cycles under some parameter conditions for $n = 3$.

On the other hand, if we allow two realistic modifications of the Lotka-Volterra system, then we can have stable limit cycles. First of all, it is unrealistic to assume that the prey grows exponentially without bounds when there is no predator. Instead, prey's growth should be limited by the carrying capacity of the environment. So x's growth rate should take the form $\alpha x(1 - \frac{x}{K})$, where K is carrying capacity. However, this is not enough since this does not go beyond the generalized Lotka-Volterra model form.

Secondly, it is unrealistic to assume that the predator's growth rate grows without bounds when the prey is unlimited, since when there are few predators and overabundant prey, the growth rate should saturate and does not increase with respect to prey's population. So the term for prey's consumption and predator's growth should take the form $\delta y \frac{x}{1+x}$. This stops increasing with x when x is much larger than 1.

Together, these modifications yield the following model:

$$\begin{aligned} \frac{d}{dt}x &= \alpha x\left(1 - \frac{x}{K}\right) - \beta y \frac{x}{1+x}, \\ \frac{d}{dt}y &= -\gamma y + \delta y \frac{x}{1+x}. \end{aligned} \tag{9}$$

This is called the Rosenzweig–MacArthur model.

Write computer code to simulate this ODE. Try it out for the following parameter set and observe a stable limit cycle. $\alpha = \gamma = 1, \beta = \delta = 3, K = 3$.

You can also play around with the parameters to see that, if we only add one of the two modifications, then the positive fixed point is always stable so the predator and prey stably co-exists.

Reference: A lecture note by Hal Smith analyzing this variant of the Lotka-Volterra model can be found at `https://sites.science.oregonstate.edu/~deleenhp/teaching/fall15/MTH427/Rosenzweig.pdf`.