Homework 3

Due Thursday 11/03/16 (9am)

4.8.6 Global dynamics from local stability analysis.

a) Consider the chemical reaction network with mass-action kinetics:

$$A + X \xrightarrow{k_1} 2X$$

$$X + X \xrightarrow{k_2} Y$$

$$Y \xrightarrow{k_3} B.$$

Assume that [A] and [B] are held constant.

- i) Write a differential equation model describing the concentrations of X and Y.
- ii) Verify that the system has two steady states.
- iii) Determine the system Jacobian at the steady states and characterize the local behavior of the system near these points.
- iv) By referring to the network, provide an intuitive description of the system behaviour starting from any initial condition for which [X] = 0.
- v) Sketch a phase portrait for the system that is consistent with your conclusions from (iii) and (iv).
- b) Repeat for the system

$$A + X \xrightarrow{k_1} 2X$$

$$X + Y \xrightarrow{k_2} 2Y$$

$$Y \xrightarrow{k_3} B.$$

In this case, you'll find that the non-zero steady-state is a center: it is surrounded by concentric periodic trajectories.

4.8.8 Linearization.

Consider the simple reaction system \rightarrow S \rightarrow , where the reaction rates are

production: V_0 consumption: $\frac{V_{\text{max}}[S]}{K_M + [S]}$.

a) Write the differential equation that describes the dynamics in s = [S]. Find the steady state. Next, approximate the original system by linearizing the dynamics around the steady state. This approximation takes the form of a linear differential equation in the new variable $x(t) = s(t) - s^{ss}$. b) Take parameter values V0 = 2, $V_{max} = 3$, and $K_M = 1$ and run simulations of the nonlinear and linearized systems starting at initial conditions [S] = 2.1, [S] = 3, and [S] = 12. Comment on the discrepancy between the linear approximation and the original nonlinear model.

4.8.13 Sensitivity analysis: reversible reaction.

Consider the reversible reaction with mass-action rate constants as shown.

$$A \stackrel{k_1}{\rightleftharpoons} A^*$$

Let T be the total concentration of A and A*.

- a) Solve for the steady-state concentration of A^* and verify that an increase in k_1 leads to an increase in $[A^*]^{ss}$.
- b) Use parametric sensitivity analysis to determine whether the steady state concentration of A* is more sensitive to a 1% increase in T or a 1% increase in k_1 . Does the answer depend on the values of the parameters?