Written Homework #7
ChE 231
Spring 2019

Problem 1. Consider the following nonlinear algebraic equation:

$$f(x) = x^2 + x - 2$$

Formulate the iterative equation for the Newton-Raphson method. Show that the method converges to a solution after 4 iterations for the initial guess $x_0 = 0$. Interpret your results in terms of the convergence properties of the method.

Problem 2. Consider a biochemical reaction network involving two intracellular species with molar concentrations S_1 and S_2. The production rate of the first species is denoted v_0. The first species inhibits its own production rate and is degraded at a constant molar reaction rate v_1. The molar rate of the reaction which produces the second species from the first species is denoted v_2. The second species is assumed to be degraded at a molar reaction rate v_3. The mass balance equations describing the reaction network are:

$$\begin{aligned}
\frac{dS_1}{dt} &= v_0 - v_1 - v_2 = k_0 \frac{K}{K + S_1} - v_1 - k_2 S_1 = f_1(S_1) \\
\frac{dS_2}{dt} &= v_2 - v_3 = k_2 S_1 - k_3 S_2 = f_2(S_1, S_2)
\end{aligned}$$

where k_0, k_2, and k_3 are reaction rate constants and K is an inhibition constant.

1. Given the following parameter values $k_0 = 4.5$, $K = 0.5$, $v_1 = 0.5$, $k_2 = 1$, and $k_3 = 1$, show that $\bar{S}_1 = \bar{S}_2 = 1$ is the single physically meaningful steady state.

2. Linearize the nonlinear model equations about the steady given in part 1. Show that linearized model can be written as:

$$\begin{aligned}
\frac{dS_1'}{dt} &= -2S_1' \\
\frac{dS_2'}{dt} &= S_1' - S_2'
\end{aligned}$$

where $S_1'(t) = S_1(t) - \bar{S}_1$ and $S_2'(t) = S_2(t) - \bar{S}_2$.

3. Show that the linearized model has the following eigenvalues and eigenvectors:

$$\lambda_1 = -2, \mathbf{x}^{(1)} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}; \qquad \lambda_2 = -1, \mathbf{x}^{(2)} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

   Examine the eigenvalues to determine if the steady state is locally asymptotically stable.

4. Consider the initial conditions $S_1(0) = 5$ and $S_2(0) = 2$. Use the eigenvalues and eigenvectors given in part 3 to determine the solution $S_1(t)$ and $S_2(t)$. Does this solution represent an exact solution for the original nonlinear model?

5. Consider the original nonlinear model. Develop the iterative equations for numerical solution by the backward difference Euler method. Propose a solution procedure for these implicit equations.