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.

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

$$x_{n+1} = x_n - \frac{f(x_n)}{\frac{\partial f}{\partial x}(x_n)} = x_n - \frac{x_n^2 + x_n - 2}{2x_n + 1}$$

$$x_{n+1} = \frac{x_n(2x_n + 1) - x_n^2 - x_n + 2}{2x_n + 1} = \frac{x_n^2 + 2}{2x_n + 1}$$

n	x_n
0	0
1	2
2	1.20
3	1.01
4	1.00

$f(1) = (1)^2 + 1 - 2 = 0$

$\Rightarrow x = 1$ is a solution

$f(x)$ is 3 times differentiable

$\frac{df}{dx} + \frac{d^2f}{\partial x^2} \neq 0$ at $x = 1$

$x_0 = 0$ is "close" to $x = 1$

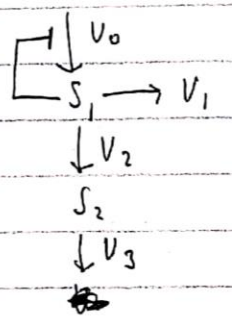
$\Rightarrow$ quadratic convergence. $|\varepsilon_{n+1}| = c|\varepsilon_n|^2$

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.



$$\frac{dS_1}{dt} = V_0 - V_1 - V_2 = k_0 \frac{K}{K+S_1} - V_1 - k_2 S_1$$

$$\frac{dS_2}{dt} = V_2 - V_3 = k_2 S_1 - k_3 S_2$$

$k_0 = 4.5$, $K = 0.5$, $V_1 = 0.5$, $k_2 = 1$, $k_3 = 1$

$$0 = k_0 \frac{K}{K + \bar{S}_1} - V_1 - k_2 \bar{S}_1 = \frac{2.25}{0.5 + \bar{S}_1} - 0.5 - \bar{S}_1$$

$$\Rightarrow 2.25 - 0.5(0.5 + \bar{S}_1) - (0.5 + \bar{S}_1)\bar{S}_1 = 0$$

$$\Rightarrow -\bar{S}_1^2 - \bar{S}_1 + 2 = 0 \Rightarrow \bar{S}_1^2 + \bar{S}_1 - 2 = (\bar{S}_1 - 1)(\bar{S}_1 + 2) = 0$$

$\bar{S}_1 = +1$ OK $\qquad \bar{S}_1 = -2$ not physically meaningful

$$0 = k_2 \bar{S}_1 - k_3 \bar{S}_2 \Rightarrow \bar{S}_2 = \frac{k_2}{k_3}\bar{S}_1 = \frac{1}{1}(1) = 1$$

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

$$\frac{dS_1'}{dt} = -2S_1'$$
$$\frac{dS_2'}{dt} = S_1' - S_2'$$

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

$$\frac{dS_1}{dt} = f_1(S_1) \qquad S_1' \equiv S_1 - \bar{S}_1$$

$$\frac{dS_2}{dt} = f_2(S_1, S_2) \qquad S_2' \equiv S_2 - \bar{S}_2$$

$$\frac{dS_1'}{dt} = \cancelto{0}{f_1(\bar{S}_1)} + \left.\frac{\partial f_1}{\partial S_1}\right|_{\bar{S}_1} S_1' = \left[-k_0 \frac{k}{(k+\bar{S}_1)^2} - k_1\right] S_1'$$

$$\frac{dS_1'}{dt} = \left[-(4.5)\frac{(0.5)}{(0.5+1)^2} - 1\right] S_1' = -2S_1'$$

$$\frac{dS_2'}{dt} = \cancelto{0}{f_2(\bar{S}_1, \bar{S}_2)} + \left.\frac{\partial f_2}{\partial S_1}\right|_{\bar{S}_1, \bar{S}_2} S_1' + \left.\frac{\partial f_2}{\partial S_2}\right|_{\bar{S}_1, \bar{S}_2} S_2'$$

$$= k_1 S_1' - k_2 S_2' = (1) S_1' - (1) S_2' = S_1' - S_2'$$

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.

$$x \equiv \begin{bmatrix} s_1' \\ s_2' \end{bmatrix} \qquad \frac{dx}{dt} = \begin{bmatrix} -2 & 0 \\ 1 & -1 \end{bmatrix} x = Ax$$

A lower triangular $\Rightarrow \lambda_1 = a_{11} = -2, \ \lambda_2 = a_{22} = -1$

$Re(\lambda_i) < 0 \Rightarrow$ System is stable.

$$Ax = \lambda x \Rightarrow \begin{bmatrix} -2 & 0 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} \lambda x_1 \\ \lambda x_2 \end{bmatrix} = 0$$

$$\Rightarrow -(2+\lambda)x_1 + 0x_2 = 0$$
$$x_1 - (1+\lambda)x_2 = 0$$

$$\lambda_1 = -2 \Rightarrow \begin{matrix} 0x_1 + 0x_2 = 0 \\ x_1 + x_2 = 0 \end{matrix} \Rightarrow x^{(1)} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

$$\lambda_2 = -1 \Rightarrow \begin{matrix} -x_1 + 0x_2 = 0 \\ x_1 + 0x_2 = 0 \end{matrix} \Rightarrow x_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

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?

$$x(t) = c_1 x^{(1)} e^{\lambda_1 t} + c_2 x^{(2)} e^{\lambda_2 t}$$

$$= c_1 \begin{bmatrix} -1 \\ 1 \end{bmatrix} e^{-2t} + c_2 \begin{bmatrix} 0 \\ 1 \end{bmatrix} e^{-t}$$

$$\begin{bmatrix} S_1(t) \\ S_2(t) \end{bmatrix} = \begin{bmatrix} \bar{S}_1 \\ \bar{S}_2 \end{bmatrix} + x(t) = \begin{bmatrix} 1 \\ 1 \end{bmatrix} + c_1 \begin{bmatrix} -1 \\ 1 \end{bmatrix} e^{-2t} + c_2 \begin{bmatrix} 0 \\ 1 \end{bmatrix} e^{-t}$$

$$\begin{bmatrix} S_1(0) \\ S_2(0) \end{bmatrix} = \begin{bmatrix} 5 \\ 2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} + c_1 \begin{bmatrix} -1 \\ 1 \end{bmatrix} + c_2 \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\Rightarrow 5 = 1 - c_1 \Rightarrow c_1 = -4$$

$$\Rightarrow 2 = 1 + (-4)(1) + c_2 \Rightarrow c_2 = 5$$

$$\begin{bmatrix} S_1(t) \\ S_2(t) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} - 4 \begin{bmatrix} -1 \\ 1 \end{bmatrix} e^{-2t} + 5 \begin{bmatrix} 0 \\ 1 \end{bmatrix} e^{-t}$$

Solution not exact - based on linearized 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.

$$S_{1,n+1} = S_{1,n} + h\left[k_0 \frac{K}{K + S_{1,n+1}} - V_1 - k_2 S_{1,n+1}\right] \Rightarrow$$ quadratic eqn for $S_{1,n+1}$

$$S_{2,n+1} = S_{2,n} + h\left[k_2 S_{1,n+1} - k_3 S_{2,n+1}\right] \Rightarrow$$ linear eqn for $S_{2,n+1}$

Solution procedure: 1) Given $S_{1,n}$, solve quadratic eqn for $S_{1,n+1}$

2) Given $S_{2,n}$ and $S_{1,n+1}$ solve linear eqn for $S_{2,n+1}$

3) Iterate