Fall 2002. 10.34. Numerical Methods Applied to Chemical Engineering

Exam I. 10/4/2002

SOLUTION

Question 1. 60 points total

Consider the following set of three nonlinear algebraic equations,

$$\begin{aligned} f_1(x_1, x_2, x_3) &= 4x_1^4 - 3x_1x_2^2 + x_2x_3 - 57 = 0 \\ f_2(x_1, x_2, x_3) &= x_2^4 - 5x_1x_3 + 9 = 0 \\ f_3(x_1, x_2, x_3) &= 3x_3^4 + 6x_1x_2x_3 - 15 = 0 \end{aligned} \qquad \text{(EQ 1)}$$

1.A. (15 pts.) Calculate the analytical form of the Jacobian matrix of this system, expressed in terms of the unknowns x_1, x_2, x_3.

Answer

The analytical form of the Jacobian matrix is

$$J = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} \end{bmatrix} = \begin{bmatrix} (16x_1^3 - 3x_2^2) & (-6x_1x_2 + x_3) & x_2 \\ -5x_3 & 4x_2^3 & -5x_1 \\ 6x_2x_3 & 6x_1x_3 & (12x_3^3 + 6x_1x_2) \end{bmatrix}$$

1.B. (10 pts.) Starting from an initial guess of $x_1 = 1$, $x_2 = 1$, $x_3 = 1$, derive the set of linear algebraic equations that must be solved for the first iteration of Newton's method.

Answer

The initial guess vector, and the value of the function vector for the initial guess, are

$$\underline{x}^{[0]} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \qquad \underline{f}^{[0]} = \underline{f}(\underline{x}^{[0]}) = \begin{bmatrix} -55 \\ 5 \\ -6 \end{bmatrix}$$

The Jacobian, evaluated at the initial guess, is

$$J^{[0]} = \begin{bmatrix} 13 & -5 & 1 \\ -5 & 4 & -5 \\ 6 & 6 & 18 \end{bmatrix}$$

The system of equations to solve for the Newton's method update is

$$J^{[0]}\Delta x^{[0]} = -f^{[0]}$$

$$\begin{bmatrix} 13 & -5 & 1 \\ -5 & 4 & -5 \\ 6 & 6 & 18 \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \Delta x_3 \end{bmatrix} = \begin{bmatrix} 55 \\ -5 \\ 6 \end{bmatrix}$$

1.C. (20 pts.) Solve this set of equations for the full Newton update $\Delta x^{[0]}$ using Gaussian elimination with partial pivoting. Show ***all*** of your calculations by hand, and use the exact solution process followed by a computer (no human intuition, please!).

*You will not receive full credit unless you show all of your calculations as performed by hand. This is to avoid giving an unfair advantage to those with fancy calculators. You **may** use a calculator, however, to add or multiply simple numbers, e.g. 5 - 4*2.*

Answer

To perform Gaussian elimination, we put the linear system in augmented matrix form,

$$\begin{bmatrix} 13 & -5 & 1 & 55 \\ -5 & 4 & -5 & -5 \\ 6 & 6 & 18 & 6 \end{bmatrix}$$

First, we zero the elements in the first column. Since the (1,1) element is largest in magnitude of any elements in the first column, no pivoting is required for this column. We zero the (2,1) elements by performing the row operation

$$\lambda_{21} = \frac{a_{21}}{a_{11}} = \frac{-5}{13} \qquad a_{2j} \leftarrow a_{2j} - \lambda_{21} a_{1j} \qquad b_2 \leftarrow b_2 - \lambda_{21} b_1$$

This yields the modified system of equations

$$\begin{bmatrix} 13 & -5 & 1 & 55 \\ 0 & 2.0769 & -4.6154 & 16.1538 \\ 6 & 6 & 18 & 6 \end{bmatrix}$$

Next, we zero the (3,1) element with the row operation

$$\lambda_{31} = \frac{a_{31}}{a_{11}} = \frac{6}{13} \qquad a_{3j} \leftarrow a_{3j} - \lambda_{31} a_{1j} \qquad b_3 \leftarrow b_3 - \lambda_{31} b_1$$

to yield

$$\begin{bmatrix} 13 & -5 & 1 & 55 \\ 0 & 2.0769 & -4.6154 & 16.1538 \\ 0 & 8.3077 & 17.5385 & -19.3840 \end{bmatrix}$$

We next move to the second column, and note that a pivot operation is required to exchange the second and third rows.

$$\begin{bmatrix} 13 & -5 & 1 & 55 \\ 0 & 8.3077 & 17.5385 & -19.3840 \\ 0 & 2.0769 & -4.6154 & 16.1538 \end{bmatrix}$$

We now zero the (3,2) element by performing the row operation

$$\lambda_{32} = \frac{a_{32}}{a_{22}} = \frac{2.0769}{8.3077} \qquad a_{3j} \leftarrow a_{3j} - \lambda_{32} a_{2j} \qquad b_3 \leftarrow b_3 - \lambda_{32} b_2$$

to yield

$$\begin{bmatrix} 13 & -5 & 1 & 55 \\ 0 & 8.3077 & 17.5385 & -19.3840 \\ 0 & 0 & -9.0000 & 21.0000 \end{bmatrix}$$

This yields an upper triangular system of equations that can be solved using backward substitution.

$$\begin{bmatrix} 13 & -5 & 1 \\ 0 & 8.3077 & 17.5385 \\ 0 & 0 & -9.0000 \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \\ \Delta x_3 \end{bmatrix} = \begin{bmatrix} 55 \\ -19.3840 \\ 21.0000 \end{bmatrix}$$

$$\Delta x_3 = \frac{21.0000}{-9.0000} = -2.3333$$

$$\Delta x_2 = \frac{(-19.3840) - (17.5385)(\Delta x_3)}{8.3077} = 2.5926$$

$$\Delta x_1 = \frac{55 - (1)(\Delta x_3) - (-5)(\Delta x_2)}{13} = 5.4074$$

1.D. (15 pts.) We have seen that Newton's method can be erratic when the initial guess is far away from the solution. If you were using a modification of Newton's method that was more robust to the choice of initial guess, would you accept the Newton update $\Delta x^{[0]}$ that you have calculated above?

If not, explain briefly how you would go about selecting the new estimate of the solution, $x^{[1]}$.

Answer

From our calculations above, the new estimate of the solution using the full Newton update step is

$$\underline{x}^{[1]} = \underline{x}^{[0]} + \Delta\underline{x}^{[0]} = \begin{bmatrix} 6.4074 \\ 3.5926 \\ -1.3333 \end{bmatrix}$$

At this new estimate, the function value is

$$\underline{f}^{[1]} = \underline{f}(\underline{x}^{[1]}) = \begin{bmatrix} 6432.1 \\ 218.3 \\ -189.7 \end{bmatrix}$$

If we compute the 2-norms of these two function vectors, we see that

$$\left\|\underline{f}^{[1]}\right\|_2 = \sqrt{\underline{f}^{[1]} \bullet \underline{f}^{[1]}} = 6438.6 \qquad \left\|\underline{f}^{[0]}\right\|_2 = \sqrt{\underline{f}^{[0]} \bullet \underline{f}^{[0]}} = 55.5518$$

Therefore, the new estimate has a function vector of even larger magnitude than the initial guess, and is in this sense a worse estimate of the solution, for which the function vector is exactly zero. We would therefore ***NOT*** accept this new estimate.

Instead, we would generate a new estimate of the solution by performing a weak line-search (the reduced-Newton method). We would search the sequence of values

$$\lambda^{[0]} = 2^{-m} \qquad m = 0, 1, 2, 3, \ldots$$

where we accept the first value of $\lambda^{[0]}$ generated by this sequence that satisfies

$$\left\| \underline{f}(\underline{x}^{[0]} + \lambda^{[0]} \Delta \underline{x}^{[0]}) \right\|_2 < \left\| \underline{f}^{[0]} \right\|_2$$

We then take as the new estimate of the solution

$$\underline{x}^{[1]} = \underline{x}^{[0]} + \lambda^{[0]} \Delta \underline{x}^{[0]}$$

Since we are choosing $\Delta \underline{x}^{[0]}$ from the solution of $J^{[0]} \Delta x^{[0]} = -\underline{f}^{[0]}$, it can be shown that unless the Jacobian is singular, there must be some positive value of $\lambda^{[0]}$ that satisfies this condition.

If we perform this weak line search at every step, we always reduce the magnitude of the norm of the function vector - a quantity that has a global minimum at a solution where the function vector and its norm are zero. This technique is robust, because we will either find a solution (desired outcome) or we will find a local minimum of the norm that is not a solution (the function vector is zero). We have shown that this can only occur if the Jacobian is singular.

If the latter outcome occurs, we can try different initial guesses. Unfortunately, with a nonlinear set of equations, it is not possible in general to say whether there exists any solution.

(QUESTION 2 ON NEXT PAGE)

Question 2. 40 points total

As we discussed in class, eigenvalue analysis can be used to study the stability of a dynamic system. If we have a system governed by a system of differential equations

$$\begin{aligned} \frac{dx_1}{dt} &= \dot{x}_1 = f_1(x_1, x_2, \ldots, x_N) \\ \frac{dx_2}{dt} &= \dot{x}_2 = f_2(x_1, x_2, \ldots, x_N) \\ &\vdots \\ \frac{dx_N}{dt} &= \dot{x}_N = f_N(x_1, x_2, \ldots, x_N) \end{aligned} \qquad \text{(EQ 2)}$$

with a steady state at $\underline{x} = \hat{\underline{x}}$, that is,

$$f_j(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_N) = 0 \qquad j = 1, 2, \ldots, N \qquad \text{(EQ 3)}$$

then the condition that the steady state be stable is that **ALL** eigenvalues of the Jacobian,

$$J_{jk}(\hat{x}) = \left.\frac{\partial f_j}{\partial x_k}\right|_{x = \hat{x}} \qquad \text{(EQ 4)}$$

must have real parts less than zero.

$$J\underline{w}^{[j]} = \lambda_j \underline{w}^{[j]} \qquad Re(\lambda_j) < 0 \qquad j = 1, 2, \ldots, N \qquad \text{(EQ 5)}$$

The full details of the derivation are repeated for your review *(should not be needed to solve the problem)* in the optional background section following the problem statement.

Consider the case of a CSTR with the single chemical reaction,

$$A + B \rightarrow 2A \qquad r = kc_A c_B \qquad \text{(EQ 6)}$$

For example, this model may describe the increase in cell concentration (species *A*) in a bioreactor containing a growth factor (species *B*). Since we see that the reaction is self-accelerating, we might be concerned about the stability of this reactor system.

The mass balances for the reactor are

$$\begin{aligned} \frac{d}{dt}[Vc_A] &= Qc_A^{(in)} - Qc_A + Vkc_A c_B \\ \frac{d}{dt}[Vc_B] &= Qc_B^{(in)} - Qc_B - Vkc_A c_B \end{aligned} \qquad \text{(EQ 7)}$$

Q is the volumetric flow rate through the reactor, V is the total reactor volume, and $c_A^{(in)}$ and $c_B^{(in)}$ are the inlet concentrations of *A* and *B* respectively. Defining the reactor mean residence time as $\theta = V/Q$, the two nonlinear equations for the steady state are

$$\begin{aligned} 0 &= c_A^{(in)} - c_A + \theta k c_A c_B \\ 0 &= c_B^{(in)} - c_B - \theta k c_A c_B \end{aligned} \qquad \text{(EQ 8)}$$

We can easily solve these equations by adding them to obtain the relation

$$\begin{aligned} 0 &= c_A^{(in)} + c_B^{(in)} - c_A - c_B \\ c_B &= c_A^{(in)} + c_B^{(in)} - c_A \end{aligned} \qquad \text{(EQ 9)}$$

Substitution into the balance for A yields

$$\begin{aligned} 0 &= c_A^{(in)} - c_A + \theta k c_A [c_A^{(in)} + c_B^{(in)} - c_A] \\ 0 &= c_A^{(in)} - c_A + \theta k c_A [c_A^{(in)} + c_B^{(in)}] - \theta k c_A^2 \\ \theta k c_A^2 &+ [1 - \theta k [c_A^{(in)} + c_B^{(in)}]] c_A - c_A^{(in)} = 0 \end{aligned} \qquad \text{(EQ 10)}$$

This quadratic equation is solved easily for the concentration of *A*.

For the process conditions,

$$\theta = 10 \qquad k = 1 \qquad c_A^{(in)} = 1 \qquad c_B^{(in)} = 10 \qquad \text{(EQ 11)}$$

the concentrations of *A* and *B* in the reactor at steady state are

$$c_A = 10.9092 \qquad c_B = 0.0908 \qquad \text{(EQ 12)}$$

2.A. (20 pts.). Is the reactor stable under these process conditions?

Answer

To determine the stability of this steady state, we must find whether all eigenvalues have a real part less than zero.

First, we define the state variables

$$x_1 = c_A \qquad x_2 = c_B$$

Then the set of differential equations, in the standard form shown above is

$$\frac{dc_A}{dt} = \theta^{-1}c_A^{(in)} - \theta^{-1}c_A + kc_Ac_B = f_1(x_1, x_2) = \theta^{-1}c_A^{(in)} - \theta^{-1}x_1 + kx_1x_2$$

$$\frac{dc_A}{dt} = \theta^{-1}c_B^{(in)} - \theta^{-1}c_B - kc_Ac_B = f_2(x_1, x_2) = \theta^{-1}c_B^{(in)} - \theta^{-1}x_2 - kx_1x_2$$

The Jacobian matrix of the system is therefore

$$J = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} = \begin{bmatrix} (-\theta^{-1} + kx_2) & kx_1 \\ -kx_2 & (-\theta^{-1} - kx_1) \end{bmatrix}$$

At the steady state conditions

$$\theta^{-1} = 0.1 \qquad k = 1 \qquad x_1 = 10.9092 \qquad x_2 = 0.0908$$

the Jacobian takes the numerical value

$$J = \begin{bmatrix} -0.0092 & 10.9092 \\ -0.0908 & -11.0092 \end{bmatrix}$$

We now have to compute the eigenvalues of this matrix. We generate the characteristic polynomial, $p(\lambda) = det(J - \lambda I)$, and solve the quadratic polynomial analytically. The results of this calculation were presented in the class notes in the form,

$$\lambda_{1,2} = \frac{T \pm \sqrt{T^2 - 4D}}{2}$$

where

$$T = tr(J) = J_{11} + J_{22} = -11.0183$$

$$D = det(J) = J_{11}J_{22} - J_{21}J_{12} = 1.0918$$

This yields the two eigenvalues of the Jacobian

$$\lambda_1 = -0.1000 \qquad \lambda_2 = -10.9183$$

Since both of these eigenvalues have real parts that are less than zero, we see that this steady state is stable.

2.B. (15 pts.). This application of eigenvalue analysis assumes that the eigenvectors of the Jacobian are linearly independent, so that any vector may be written as a linear combination of the eigenvectors. While this assumption is usually OK, we can only *prove* that it is valid for special cases of the Jacobian matrix J and of its eigenvalues $\lambda_1, \lambda_2, ..., \lambda_N$.

What are the most general conditions on J and $\lambda_1, \lambda_2, ..., \lambda_N$ that you can impose for the eigenvectors of J to be linearly independent?

Answer

The $N \times N$ matrix J has a linearly independent set of eigenvectors if any of the following two conditions holds

I. All N eigenvalues of J are distinct; that is, $\lambda_1 \neq \lambda_2 \neq \lambda_3 \neq ... \neq \lambda_N$

OR

II. The matrix J is normal; that is, $JJ^T = J^TJ$

2.C. (5 pts.). For the Jacobian matrix that you calculate in 2.A, are the eigenvectors expected to be orthogonal to each other?

Answer

We can only expect the eigenvectors to be orthogonal when the matrix is normal. First, we can see from inspection that the real matrix J is not symmetric. This suggests that the matrix is not normal, but to be sure, we compare the products JJ^T and J^TJ. The matrix and its transpose are

$$J = \begin{bmatrix} -0.0092 & 10.9092 \\ -0.0908 & -11.0092 \end{bmatrix} \qquad J^T = \begin{bmatrix} -0.0092 & -0.0908 \\ 10.9092 & -11.0092 \end{bmatrix}$$

We now compute the (1,1) elements of JJ^T and J^TJ.

$$(JJ^T)_{11} = J_{11}J_{11}^T + J_{12}J_{21}^T = 119.0107$$
$$(J^TJ)_{11} = J_{11}^TJ_{11} + J_{12}^TJ_{21} = 0.0083$$

Since these two elements are not equal, we can immediately see that the matrix is not normal, $JJ^T \neq J^TJ$. Therefore, we do not expect the eigenvectors to be orthogonal.