10.34 Numerical Methods Applied to Chemical Engineering

Quiz 1

- This quiz consists of three problems worth 20, 40 and 40 points respectively. The problem statements are found on pages 2, 3 and 5 in this exam packet.
- You have 2 hours to complete the quiz.
- You are free to use a calculator or any notes you brought with you.
- It is important, however, that only the scientific – arithmetic and trigonometric – function of the calculator is used throughout the quiz. You are on your honor not to employ any built-in numerical linear algebra routines. This includes but is not limited to the calculation of determinants, eigenvalues, eigenvectors and solutions of linear equations.
- The ends of problems 2 and 3 provide an opportunity to do a little more work and earn 2 *bonus* points each. Be sure to complete the rest of the quiz before attempting these.

Problem 1 (20 points)–

1. (4 points) Create a real 2×2 matrix with a determinant and trace equal to 0 that is not the zero matrix (or explain why this is impossible)

2. (4 points) Create a real 3×3 matrix with a determinant and trace equal to 6 (or explain why this is impossible)

3. (6 points) Create a real 4×4 matrix with rank 2. Propose a vector $\mathbf{b} \in \mathbb{R}^4$ such that the system of equations $\mathbf{Ax} = \mathbf{b}$ has a family solutions. What is that family of solutions? Propose a vector $\mathbf{b} \in \mathbb{R}^4$ such that the system of equations $\mathbf{Ax} = \mathbf{b}$ has no solutions. Explain why this is the case.

4. (6 points) Notice that vectors from the null space of your matrix are orthogonal to the rows of that matrix. This is a general property of matrices which you will prove now. In particular, for a matrix $\mathbf{A} \in \mathbb{R}^{N \times M}$, prove that vectors from the null space, $\mathcal{N}(\mathbf{A})$, are orthogonal to vectors from the row space, $\mathcal{R}(\mathbf{A}^T)$.

Problem 2 (40 points) –

Problem statement:

Biological signaling and regulation networks often involve *cycles* in which a protein backbone is transformed through a collection of modified states with different numbers of phosphate groups attached. A basic cycle might be described by the reaction network:

$$\mathrm{A} \overset{k_1}{\to} \mathrm{B} \overset{k_2}{\to} \mathrm{C} \overset{k_3}{\to} \mathrm{A},$$

where A, B and C have the same protein backbone with different numbers of phosphate groups. Of course, some kind of energy input is required to maintain a cycle, which is not represented above.

Questions to be answered:

1. (2 points) Write down the stoichiometry matrix **S** for this reaction network.
2. (5 points) Characterize the null space of **S** in terms of a dimension and a basis. What does this tell you about the fluxes (reaction rates) in the network at steady state? What physical interpretation can you provide for this?
3. (5 points) Characterize the left null space of **S** in terms of a dimension and a basis. What does this tell you about the time evolution of the protein concentrations? What physical interpretation can you provide for this?
4. (5 points) Write down a model for the dynamics of the protein concentrations in a compartment of a mammalian cell using matrix-vector notation. State any assumptions in your model.
5. (8 points) Let $k_1 = 1$, $k_2 = 2$ and $k_3 = 1$. Does your model admit a steady-state solution? If so, describe it physically? Is that solution stable?

Now let us consider a cycle of length N

$$\mathrm{A} \xrightarrow{k_1} \mathrm{B} \xrightarrow{k_2} \mathrm{C} \xrightarrow{k_3} \mathrm{D} \xrightarrow{k_4} \cdots \xrightarrow{k_N} \mathrm{A},$$

6. (5 points) Sketch the sparsity pattern of the stoichiometry matrix **S** for this N component cyclic system.
7. (5 points) Write a MATLAB®function that takes advantage of this sparsity pattern to compute the product of **S** with a vector. Your function should take as an input the fluxes associated with each reaction in the cycle and return the rate of change for the concentration of each species in the cycle. Be sure that your function does not compute the stoichiometry matrix explicitly.
8. (5 points) Develop an expression for the characteristic polynomial of the N component stoichiometry matrix, **S**. The roots represent the eigenvalues of **S**.

Problem 3 (40 points) –

Problem statement:

An autocatalytic reaction converts A to B as

$$\mathrm{A} + 2\mathrm{B} \rightarrow 3\mathrm{B}.$$

The reaction is elementary so the net rates of consumption/formation of A and B are

$$r_A = -r_B = -k[A][B]^2.$$

where k is the rate constant.

If the reaction takes place in an isothermal, continuously stirred tank, the concentrations of species A and B exiting the reactor at time t, denoted C_A and C_B, satisfy the equation:

$$\frac{d}{dt}\begin{pmatrix} C_A \\ C_B \end{pmatrix} = \begin{pmatrix} \theta^{-1}\left(C_{A,f} - C_A\right) - kC_AC_B^2 \\ \theta^{-1}\left(C_{B,f} - C_B\right) + kC_AC_B^2 \end{pmatrix}. \tag{1}$$

Here, θ is the residence time in the reactor and $C_{A,f}$ and $C_{B,f}$ are the concentrations of species A and B fed to the reactor. We seek the concentrations of A and B in the effluent when the reactor reaches steady-state: $dC_A/dt = dC_B/dt = 0$.

Problem 3 (cont.) –

Questions to be answered:

1. (4 points) Show that at steady-state, equation 1 can be written as a system of nonlinear equations:

$$0 = \mathbf{f}(\hat{C}_A, \hat{C}_B) = \begin{pmatrix} \alpha\left(1 - \hat{C}_A\right) - \hat{C}_A\hat{C}_B^2 \\ \alpha\left(\beta - \hat{C}_B\right) + \hat{C}_A\hat{C}_B^2 \end{pmatrix}, \tag{2}$$

   where $\hat{C}_A = C_A/C_{A,f}$, $\hat{C}_B = C_B/C_{A,f}$, $\alpha = (k\theta C_{A,f}^2)^{-1}$, and $\beta = C_{B,f}/C_{A,f}$. This dimensionless form of the species balance at steady-state will prove useful in the remainder of the problem.

2. (10 points) Calculate the Jacobian, $\mathbf{J}_f(\hat{C}_A, \hat{C}_B)$, of the vector-valued function, $\mathbf{f}(\hat{C}_A, \hat{C}_B)$, from equation 2. Under what conditions (α, β, $\hat{C}_A$, $\hat{C}_B$) will the Jacobian be singular? Assume these quantities take on physical values – that is, they are real and non-negative. In each of those circumstances, find a vector that belongs to the null space of the Jacobian.

3. (8 points) When $\beta = 0$, no B is fed to the reactor and no A is converted. Therefore, the steady-state concentrations are $\hat{C}_A = 1$, $\hat{C}_B = 0$. Sketch an algorithm that would use this information to accelerate a search for the steady state solution at another value of the parameters (α, β), say $(1, 1)$.

4. (10 points) In a CSTR, an autocatalytic reaction can exhibit multiple steady-states. The steady-state mass balance requires that: $C_{A,f} + C_{B,f} = C_A + C_B$. This can be used to recast equation 2 as a single, cubic equation for the steady-state concentration of A or B, which may admit as few as one and as many as three solutions depending on the values of the parameters α and β. There may be a connected set of points (α, β) at which this bifurcation occurs. Describe in detail a computational approach to finding the elements of this parameter set – that is, an algorithm to search for values of α, β at which the CSTR begins to possess multiple steady states.

5. (8 points) When $(\alpha, \beta) = (1, 1)$, Newton's method converges to the solution: $\hat{C}_A^* = 0.2451$, $\hat{C}_B^* = 1.7549$. You will evaluate the stability of this steady state solution to the ODE:

$$\frac{d}{d\hat{t}}\begin{pmatrix} \hat{C}_A \\ \hat{C}_B \end{pmatrix} = \mathbf{f}(\hat{C}_A, \hat{C}_B). \tag{3}$$

   Use a Taylor expansion about the steady state solution to show that:

$$\frac{d}{d\hat{t}}\begin{pmatrix} \hat{C}_A - \hat{C}_A^* \\ \hat{C}_B - \hat{C}_B^* \end{pmatrix} = \mathbf{J}_f(\hat{C}_A^*, \hat{C}_B^*)\begin{pmatrix} \hat{C}_A - \hat{C}_A^* \\ \hat{C}_B - \hat{C}_B^* \end{pmatrix}, \tag{4}$$

   when $\|(\hat{C}_A - \hat{C}_A^*, \hat{C}_B - \hat{C}_B^*)\|_p \Rightarrow 0$. Use this linear equation to evaluate the stability of the steady state solution. Under what conditions can this result be expected to hold?

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Fall 2015