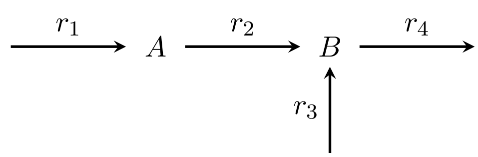
BIOE 210, SPRING 2020

HOMEWORK 2

Due Friday, 3/6/2020 before 9:00am.
Upload a single PDF with your answers to Gradescope.

Part I (20 points)

In this problem you will use a technique called Flux Balance Analysis to analyze chemical reaction networks. You will find fluxes (or *rates*) for multiple reactions that satisfy the conservation of mass. Consider the four reaction network below:



The metabolites A and B are produced and consumed by four reactions. The rates of the reactions are the unknowns $r_1, \ldots, r_4$. It is convenient to think of the four individual rates as entries in a four-dimensional flux vector $\mathbf{r}$. The connectivity of a network is captured by a *stoichiometric matrix* $\mathbf{S}$.

$$\mathbf{S} = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & 1 & -1 \\ 1 & 0 & 1 & -1 \\ 0 & -1 & -1 & 1 \end{pmatrix}$$

Conservation of mass requires that $\mathbf{Sr} = \mathbf{0}$. This homogeneous system has the trivial solution $\mathbf{r} = \mathbf{0}$, but we want to find the more interesting nontrivial solutions.

(1) Using elementary row operations, calculate the rank of $\mathbf{S}$.
(2) Find a parameterized solution for the system $\mathbf{Sr} = \mathbf{0}$.
(3) Find a specific solution for the system by choosing values for the parameters.
(4) Explain why you would expect the system to have the rank it does. Your answer should discuss the reaction network and the conservation of mass, not the linear dependence of the rows or column in $\mathbf{S}$. We want you to focus on what the rank means in terms of the dependence of the reaction rates.

Part II (10 points)

(1) The function

$$f(x) = 18x^4 + 112x^3 + 204x^2 + 144x - 17$$

may have maxima or minima at $x = -3$, -1, and $-2/3$.

  (a) Determine if the function has a local minimum or local maximum at each point.

  (b) Can you say that one of the local minima is the global minimum? If so, what is the minimum and the argmin?

(2) Consider the linear equation $y = \frac{3}{2}x + 2$.

  (a) Write this equation in Hesse normal form ($\hat{\mathbf{a}} \cdot \mathbf{x} = d$).

  (b) Plot this line and draw (and label) $\mathbf{a}$, $\hat{\mathbf{a}}$, and d.

  (c) Find the intersection between this line and the line $-3x - 2y = -1$ using Gaussian elimination.

Part III: Nonlinear Systems (20 points)

We want to find a root for the nonlinear system

$$\mathbf{f}(\mathbf{x}) = \begin{pmatrix} x_2 \cos x_1 \\ 2x_2^2 - 1 \end{pmatrix}$$

We will use multivariate Newton's method to find a vector $\mathbf{x}$ such that $\mathbf{f}(\mathbf{x}) = 0$ starting from an initial guess $\mathbf{x}_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

(1) Write the Jacobian matrix $\mathbf{J}(\mathbf{x})$ for the systems of equations.

(2) Show that $\mathbf{x}_0$ is not already a root by verifying that $\mathbf{f}(\mathbf{x}_0) \neq \begin{pmatrix} 0 \\ 0 \end{pmatrix}$.

(3) Using Newton's method, find a new guess $\mathbf{x}_1$ using $\mathbf{x}_0$. Calculate $\mathbf{f}(\mathbf{x}_1)$.
(You are welcome to use Matlab or a calculator to invert $\mathbf{J}(\mathbf{x})$ and perform any matrix multiplications.)

(4) Repeat this two more times by finding $\mathbf{x}_2$ and $\mathbf{x}_3$. Show that the values $\mathbf{f}(\mathbf{x}_2)$ and $\mathbf{f}(\mathbf{x}_3)$ approach $\begin{pmatrix} 0 \\ 0 \end{pmatrix}$.