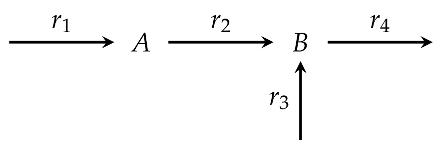
BIOE 210, Spring 2022

Homework 5

Due Monday, 2/21/2022 by 5:00pm.
You must upload your answers to Gradescope and assign each question.

1. 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.

   (a) Using elementary row operations, calculate the rank of $\mathbf{S}$.

   (b) Find a parameterized solution for the system $\mathbf{Sr} = \mathbf{0}$.

   (c) Find a specific solution for the system by choosing values for the parameters.

   (d) 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.

2. In class we derived solutions for the linear models $y = \beta_0$ and $y = \beta_0 + \beta_1 x$. Derive a least-squares solution for the one parameter, no intercept model $y = \beta_1 x$.

   (a) Write out the quadratic loss function $L(\beta_1)$ for a single data point (x_i, y_i).

   (b) Sum the loss function for a set of n data points $(x_1, y_1), \ldots, (x_n, y_n)$.

   (c) Compute the derivative of the total loss function in (b) with respect to the unknown parameter β_1.

   (d) Solve for β_1.

3. Using the solution to problem 2, fit a linear model $y = \beta_1 x$ to the data on page 59 of the textbook.