

CHEME 5440 - HW#4

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1.(a)

From $\frac{d[x^*]}{dt}=0$, $\frac{d[y^*]}{dt}=0$ and $\frac{d[R^*]}{dt}=0$ for steady-state, we get:

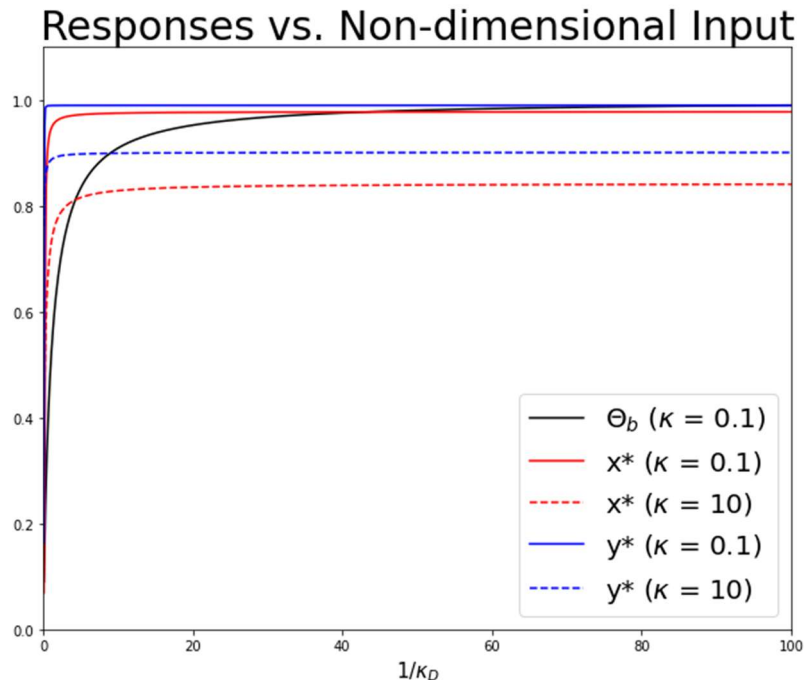
$$x^* = - \frac{1 + \kappa_1 + \frac{V_1}{V_2} \times (-1 + \kappa_2) + \sqrt{(1 + \kappa_1 + \frac{V_1}{V_2} \times (-1 + \kappa_2))^2 + 4 \times (-1 + \frac{V_1}{V_2}) \times \frac{V_1}{V_2} \times \kappa_2}}{2 \times (-1 + \frac{V_1}{V_2})}$$

$$y^* = - \frac{1 + \frac{V_3}{V_4} - \kappa_3 - \frac{V_3}{V_4} \kappa_4 + \sqrt{(1 + \kappa_3 + \frac{V_3}{V_4} \times (-1 + \kappa_4))^2 + 4 \times (-1 + \frac{V_3}{V_4}) \times \frac{V_3}{V_4} \times \kappa_4}}{2 \times (-1 + \frac{V_3}{V_4})}$$

$$\theta_B = \frac{1 - \theta_B}{\kappa_D}, \text{ thus } \theta_B = \frac{1}{1 + \kappa_D} = \frac{\frac{1}{\kappa_D}}{\frac{1}{\kappa_D} + 1}$$

1.(b)

For $\kappa_1 = \kappa_2 = \kappa_3 = \kappa_4 = \kappa$



*Code in github resp.

1.(c)

*Code in github resp.

- Did not success

1.(d)

Using `numpy.interp()`, we can obtain the y value when given a x value on a plot.

θ_B percentage change : 0.4166666666666666

x^* ($\kappa = 0.1$) percentage change : 1.4664528944969721

x^* ($\kappa = 10$) percentage change : 0.24254211403159665

y^* ($\kappa = 0.1$) percentage change : 2.3916752044004874

y^* ($\kappa = 10$)percentage change : 0.04332996901435626

*Code in github resp.

1.(e)

The consequences of zero-order sensitivity are that the signals have very sharp responses for lower values of κ ; on the other hand, there are smaller differences between input and output when the κ value increases.

2.(a)

Using Python `scipy`, we could calculate steady-state $[A]$, $[B]$ and $[C]$ without inhibitors to be approximately:

$[A] = 1.11$

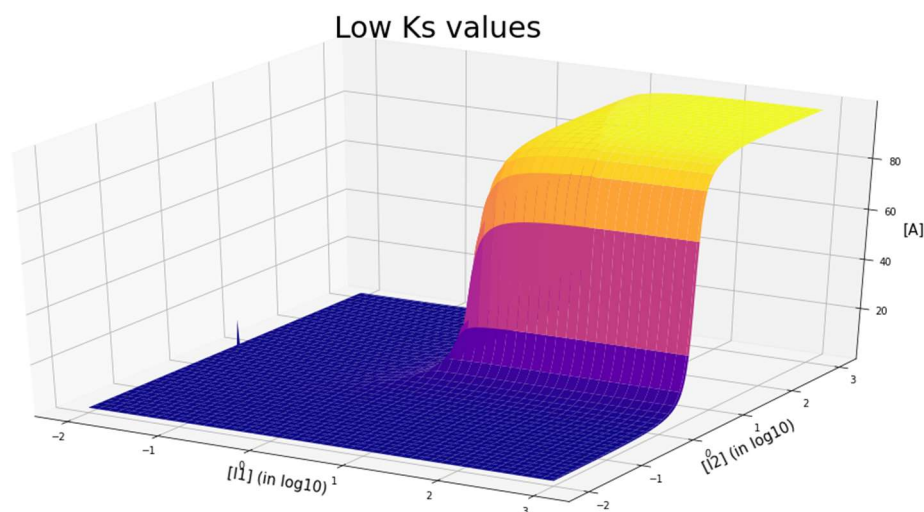
$[B] = 49.45$

$[C] = 49.45$

*Code in github resp.

2.(b)

Using Matplot, we can construct the 3D plot with a mesh of 190:



*Code in github resp.

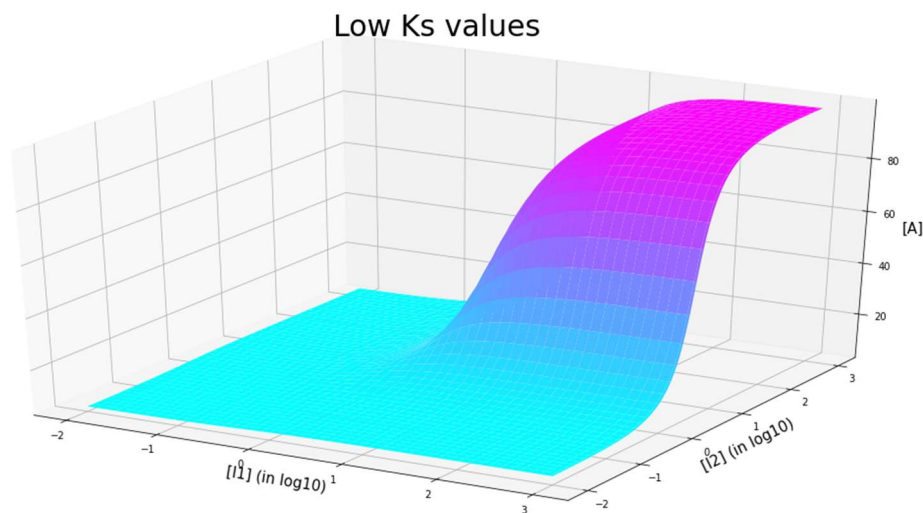
2.(c)

From part (b) plot, we can see as $[I1]$ and $[I2]$ increase, the concentration of A also increases, meaning that reactions $A \rightarrow B$ and $A \rightarrow C$ are inhibited. From part (a), we can also see that when there are no inhibitors, B and C concentrations are quite high and $[A]$ is low. However, if there is only I1, the level of A does not increase. Both I1 and I2 concentrations should be high to result in a significant increase in $[A]$.

Thus, the relationship should be an AND gate circuit, with $[I1]$ and $[I2]$ being the input and $[A]$ being the output.

2.(d)

Similar to part (b), we can construct the 3D plot while $K_{S1}=K_{S2}=K_{S3}=K_{S4}=35.0$:



*Code in github resp.

From the above plot, we can observe that the slope for the change in $[A]$ is much shallower compared to that of the plot in part (b), which could be that the gate is less sensitive and has more $[A]$ while either $[I1]$ or $[I2]$ is not at all high. This can be considered a “fuzzy” gate since the gate output results are not as definite as part (b).

2.(e)

From Goldbeter and Goshland's (1981) cell signaling work, they demonstrated that zero-order ultrasensitivity is important for tuning sharp responses. They showed that the dominant kind will have a sharp response if the K value is low, and this response is very similar to a logical gate. However, if the K value is high, then this could lead to more “fuzzy” results.