Assignment: Advanced Synthetic Biology Class 2016

Due Tuesday May 3rd

Answer the three questions.

Construct a model that includes four reversible reaction steps forming a linear chain of reactions:

$$Xo \to x_1 \to x_2 \to x_3 \to X_1$$

Assume that Xo and X1 are fixed species. Let each reaction be governed by the following reversible mass-action rate law.

$$v = k_1 (x_1 - \frac{x_2}{Keq})$$

Q1. Show that that rate laws is equivalent to $v = k_1 x_1 - k_2 x_2$ where $\frac{k_1}{k_2} - Keq$

Fix the equilibrium constants at 4, 3, 2,1 respectively for reactions v1, v2, v3, v4. Set Xo to 5.0 and X1 to 0.1

Generate 10,000 or more random models that have randomized rates constants, k1, k2, k3, and k4. For each model compute the four flux control coefficients, C_{k1}^{J} , C_{k2}^{J} , C_{k3}^{J} , C_{k4}^{J}

Q2: Draw a frequency plot of the flux control coefficients to determine the distribution of control coefficient values from the simulation.

Q3: State what you observe.

Hints: Randomize rate constants by drawing from a uniform random number distribution 0.1 to 2. It is recommended you carry out a time course simulation (ignore the output from this) in order to help the steady state solver find the solution. The simulation will generate an exception if there are any numerical errors, therefore you can use a try/except to ignore any models that don't have a steady state.

Eg

Try:

r.simulate() r.steadyState()

Do calculations

except :

fail = fail + 1 # You this is check you're not getting too many errors

Use r.getCC ('variable', 'parameter') to compute a control coefficient.

Use the matplotlib hist function to draw and bin the control coefficient values. 100 bins should work. Use an alpha channel of 0.5 so that overlapping plots don't obscure each other.