Systems Biology Tutorial 2: Chemical kinetics and energetics

Example: Reversible dissociation

Please consult the Mathematica Help Documentation and Introduction videos for the `NDSolve` and `Plot` functions. For the last question, consult the documentation for `NonlinearModelFit`.

Consider the reaction

$$A \rightleftharpoons B + C$$

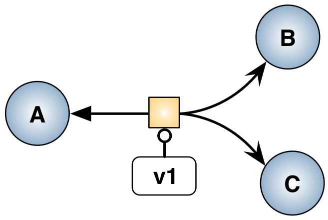

Figure 1: Graphical representation of the reversible dissociation reaction.

The change in the concentration of A is described by the ordinary differential equation (ODE)

$$\frac{dA(t)}{dt} = -v_1 \quad (1)$$

$$\text{where} \quad v_1 = k_f \cdot A(t) - k_r \cdot B(t) \cdot C(t) \quad (2)$$

1. What must the units of k_f and k_r be (if time is measured in seconds and concentration in M)?
2. Given that $k_f = 23$ and $k_r = 0.5$, write Eq. 2 in the form

$$v_1 = k_f \cdot \left(A - \frac{B \cdot C}{K_{eq}} \right) \quad (3)$$

   (a) What is the unit and value of K_{eq}?

   (b) From the information above, write the ODEs for B and C.

   (c) Solve ODEs with three variable species:

      i. For initial values $A(0) = 5$ M, $B(0) = 0$, $C(0) = 0$ and parameters as given, solve the ODEs to obtain functions for A, B and C (use `NDSolve`).

      ii. Plot the concentrations as a function of time. Plot all three solutions on the same axes in different colours. Add axis labels including units.

   (d) Solve ODEs with a fixed species:

      i. For fixed $A = 5$ M, initial values $B(0) = 0$ and $C(0) = 0$, and parameters as given, solve the ODEs to obtain functions for B and C (use `NDSolve`).
      Hint: Reduce the number of ODEs to correspond to variable species only and treat the fixed species as a parameter.

      ii. Plot the mass action ratio as a function of time. To what value does this ratio strive and why?

      iii. How does the mass action ratio change if you increase the value of k_r?

3. Use the data set provided (initial rates vs A in A.csv, and initial rates vs B and C in BC.csv) and fit a function of the form given by Eq. 2 to obtain values for k_f and k_r .

   (a) Download the two data files from the File Downloads section of the course website using your browser, and `Import` them into Mathematica.

   (b) First, fit a simplified function on the data for rate vs A to obtain k_f. The data is in the form {{A1,rate1}, {A2,rate2}, {A3,rate3}, ...}. Plot the fitted simplified rate as a function of A.

   (c) Next, fit a simplified function on the data for rate vs B and C to obtain k_r. The data is in the form {{B1,C1,rate1}, {B2,C2,rate2}, {B3,C3,rate3}, ...}. Plot the fitted simplified rate as a function of B and C using `Plot3D`.

   (d) We can, however, also fit the complete function on all of the data to obtain these parameter values. Combine the datasets into one list of the form {{A1,B1,C1,rate1}, {A2,B2,C2,rate2}, {A3,B3,C3,rate3}, ...} and fit the full function to obtain values for k_f and k_r.