Exercise for Constraint-based Modeling of Cellular Networks
1 December 2022

Homework should be sent to Anika (ankueken@uni-potsdam.de)

Hand in your commented code for all exercise tasks as homework.

Exercise

The type of coupling between two reactions i and j can be determined by solving the linear fractional program (LFP)

$$\max_{v}\,(\min)\,\frac{v_i}{v_j}$$

s.t.

$$Nv = b$$
$$\forall i, 1 \le i \le n, 0 \le v_i \le v_i^{max}$$

The LFP can be transformed into a LP, using Charnes-Cooper transformation:

$$\max_{v'}\,(\min)\,v'_i$$

s.t.

$$Nv' = bt$$
$$\forall i, 1 \le i \ne j \le n, 0 \le v'_i \le v_i^{max} t$$
$$v'_j = 1$$
$$t \ge 0$$

1) Write function C*T = coupling(model)*, that provided a metabolic model in Cobra model format calculates pairwise coupling between all n model reactions. The output *CT* is a numeric nxn double matrix with the following numbers indicating the respective type of coupling:

   0: not coupled
   1: fully coupled
   2: partially coupled
   3: directionally coupled from i to j ($v_i \ne 0 \Rightarrow v_j \ne 0$)
   4: directionally coupled from j to i ($v_j \ne 0 \Rightarrow v_i \ne 0$).

   Hint: use function round to round v' to nearest 4 decimal digits to avoid numeric problems.

   Which of the coupling types are symmetric? To improve performance, use the symmetry to avoid calculating the coupling of reaction pairs, where this is not necessary.

2) Calculate reaction coupling for the *E. coli* core model.
   For the set of fully coupled reaction pairs $\{R_i, R_j\}$, where $i \ne j$, provide a table that shows the corresponding coupling constant $\alpha_{ij} = \frac{v_i}{v_j}$, $\alpha_{ij} > 0$.