Exercise for Constraint-based Modeling of Cellular Networks

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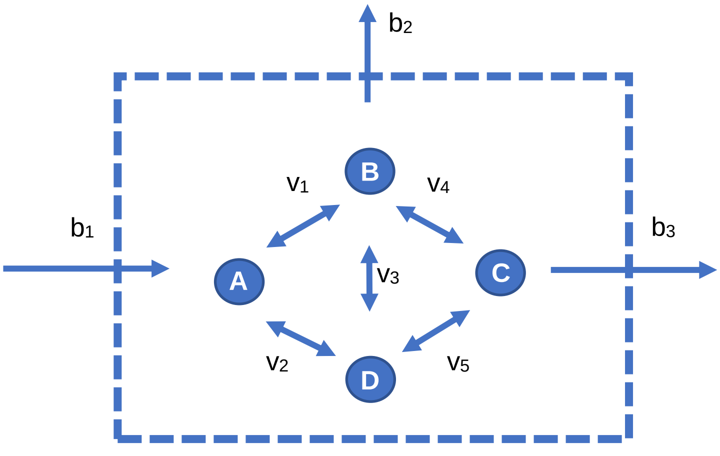
Homework should be sent to Anika (ankueken@uni-potsdam.de)

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

In the figure below a small network is illustrated, which contains five internal reactions and three exchanges. The lower bounds and upper bounds are -1000 and 1000 for internal reactions respectively, and they are 0 and 1000 for exchanges.



Exercise

1. In MATLAB, create variable N including the stoichiometric matrix for the network illustrated above. as well as LB and UB vectors including lower (v_i, min) and upper bound values (v_i, max) on reaction fluxes, respectively. (1 point)

2. Calculate $P_{int} = null(N_{int})$, the null space of the internal reactions, whose stoichiometry is given by N_{int}. (1 point)

3. With the goal of having maximum flux for the third exchange reaction, find a flux distribution which does not contain any thermodynamically infeasible reaction loop. Which reactions have non-zero values in this loop-free pathway? See lecture slide 43 for the program. Use 10^{-3} for $G_{i,min}$ and 10^{3} for $G_{i,max}$. (4 points)

4. If the ΔG^0 values for internal reactions are -2.4279e+03, -2.3289 e+03, -2.3249 e+03, 7.0838 e+03 and -4.6548 e+02 and the lower and upper bounds for metabolite concentrations are 2.5 and 200 mol/l, with the goal of maximizing the flux of third exchange reaction, find a thermodynamically feasible flux distribution compatible with Gibbs free energy and metabolite concentrations (T = 293.15 K and R = 8.3145 $J \cdot mol^{-1} \cdot K^{-1}$). See lecture slide 27 for the TMFA program. For parameter K use 10^6. (4 points)