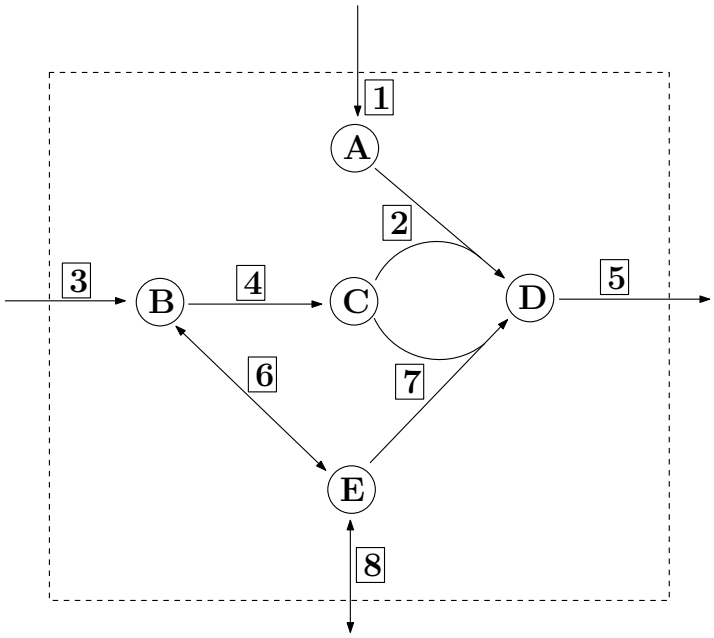
Network Analysis SS 17
Constrained-based modelling

Alexander Bockmayr
Annika Röhl

26 May 2017
Deadline: Wednesday, 7 June, 08:00 am

1 Exercise *Tutorial*

Consider the following network. Assume that all stoichiometric coefficients belong to $\{-1, 0, 1\}$.



Determine the following properties:

1. Metabolites
2. Reactions
3. Irreversible reactions
4. Stoichiometric matrix

Write down the steady-state flux cone find two valid flux vectors.

2 Exercise *Homework*

Essential reactions:

Let $S \in \mathbb{R}^{\mathcal{M}\times\mathcal{R}}$ be the stoichiometric matrix of a metabolic network, with $\mathcal{R}$ being the set of reactions and $\mathcal{M}$ being the set of metabolites. Assume we have a flux balance problem $z_{\text{opt}} = \max\{v_{\text{Biomass}} \mid Sv = 0, lb \leq v \leq ub\}$, where lb, resp. ub are the lower, resp. the upper bounds on the flux rates. We call a reaction *essential* if after removing this reaction it is no longer possible to achieve at least 20% of the maximal biomass production rate: let $z_r = \max\{v_{\text{Biomass}} \mid Sv = 0, lb \leq v \leq ub,\ v_r = 0\}$. If $z_r \leq 0.2 \cdot z_{\text{opt}}$ then r is an essential reaction.

Write a program in `MATLAB`, that:

- reads in a metabolic network: a struct in a .mat file, which is called "network":
    1. `S`: stoichiometric matrix
    2. `rev`: reversibility-vector (rev(i) = 0: reaction i is not reversible, rev(i) = 1: reaction i is reversible)
    3. `rxns`: names of the reactions
    4. `lb`: lower bounds
    5. `ub`: upper bounds
    6. `description`: name of the network

The program should iteratively compute the essential reactions.
Output:

- A `.csv` file with two columns
- in the first column are the indices of the essential reactions, in the second column are the corresponding names of the reactions.

3 Exercise *Homework*

FVA:
Write a program in `MATLAB`, that:

- reads in a metabolic network: a struct in a .mat file, which is called "network":
  1. `S`: stoichiometric matrix
  2. `rev`: reversibility-vector (rev(i) = 0: reaction i is not reversible, rev(i) = 1: reaction i is reversible)
  3. `rxns`: names of the reactions
  4. `lb`: lower bounds
  5. `ub`: upper bounds
  6. `description`: name of the network
- reads in a second argument, which is either `BIOMASS` or the name of a reaction
- reads in a third argument, which is the name of the output file.

The program should compute the flux-variability for each reaction.
Output:

- Three .txt Files which should have the name of the output file and as an addition `_variable`, `_notvariable` or `_notused`.
- `variable` file should consists of three columns:
  1. in the first column are the names of the reactions, ordered according to their index
  2. in the second column is the maximum flux through the corresponding reaction
  3. in the second column is the minimum flux through the corresponding reaction
- The title of the columns are:
  1. `Name`
  2. `Max Value`
  3. `Min Value`
- The `notvariable` file should consists of two columns:
  1. in the first column are the names of the reactions, ordered according to their index. In the first row is the biomass-reaction or the reaction which should be maximised
  2. in the second column are the fluxes for the corresponding reactions
- the `notused` file contains one column where the reaction names are listed (according to their indices) which never carry flux.

Please download these networks to test your program.

Send the programs for exercise 2 and 3 until Wednesday 7. June, 08:00 am to `Annika.Roehl@fu-berlin.de`