Constraint-based Modeling of Cellular Networks

Exercise 7 – Flux coupling

01. 12. 2022

From fractional LP to LP

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

s.t.

$$Nv = 0$$

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

$$\max_{v'} (\min) v_i{}'$$

s.t.

$$Nv' = 0$$

$$\forall i, 1 \le i \le n, 0 \le v_i' \le v_i^{max}.t$$

$$v_j' = 1$$

No more *v* variable here!

Q: How are v and v‘ related?

How can we go back to v after solving the LP?

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No more *v* variable here!

Q: How are v and v‘ related?

How can we go back to v after solving the LP?

$$v = \frac{1}{t} v‘$$

Implementing the LP

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

s.t.

$$Nv' = 0$$
$$\forall i, 1 \leq i \leq n, 0 \leq v_i' \leq v_i^{max} t$$
$$v_j' = 1$$

What is the dimension of the variable vector x when implementing the LP problem above?

General form of LP:

$$\max_{x} (\min) \, c^T x$$

s.t.

$$\mathrm{Ax} \begin{matrix} \leq \\ = \end{matrix} b$$
$$lb \leq x \leq ub$$

Implementing the LP

$$\max_{v'} (\min)\ {v_i}'$$

s.t.

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$$\forall i, 1 \leq i \leq n, 0 \leq v'_i \leq v_i^{max} t$$

$$v'_j = 1$$

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$$x = \begin{bmatrix} v'_1 \\ \vdots \\ v'_n \\ t \end{bmatrix}$$

we have n+1 variables

Implementing the LP

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

s.t.

$$Nv' = 0$$

$$\forall i, 1 \le i \le n, 0 \le v_i' \le v_i^{max} t$$

$$v_j' = 1$$

What does having n+1 variables in x mean for matrix A?

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s.t.

$$\mathrm{Ax} \underset{=}{\le} b$$

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$$x = \begin{bmatrix} v'_1 \\ \vdots \\ v'_n \\ t \end{bmatrix}$$

$$A = \overbrace{\begin{bmatrix} [N_{m\times n}] & \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} \end{bmatrix}}^{\text{n+1 columns}} \times \begin{bmatrix} v'_1 \\ \vdots \\ v'_n \\ t \end{bmatrix}$$

Implementing the LP

$$\max_{v'} (\min)\ v_i{}'$$

s.t.

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Implementing the LP

$$\forall i, 1 \leq i \leq n, 0 \leq v_i' \leq v_i^{max} t$$

$$\begin{aligned} &\max_{v'} \, (\min) \, v_i{}' \\ &\quad \text{s.t.} \\ &\qquad Nv' = 0 \\ &\qquad \forall i, 1 \leq i \leq n, 0 \leq v_i' \leq v_i^{max} t \\ &\qquad v_j' = 1 \end{aligned}$$

How can we rewrite the equation such that we can implement it?
Variables on left side and constants on right-hand side.

Implementing the LP

$$\forall i, 1 \le i \le n, 0 \le v_i' \le v_i^{max} t$$

$$v'_i - v_i^{max} t \le 0$$

$$\max_{v'} \text{ (min) } v_i'$$

s.t.

$$Nv' = 0$$

$$\forall i, 1 \le i \le n, 0 \le v_i' \le v_i^{max} t$$

$$v_j' = 1$$

Implementing the LP

$$\forall i, 1 \le i \le n, 0 \le v_i' \le v_i^{max} t$$

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s.t.

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$$\forall i, 1 \le i \le n, 0 \le v_i' \le v_i^{max} t$$

$$v_j' = 1$$

$$\left[\begin{array}{c:c} I_{n\times n} & \begin{bmatrix} -v_1^{max} \\ -v_2^{max} \\ \vdots \\ -v_n^{max} \end{bmatrix} \end{array}\right] \times \begin{bmatrix} v'_1 \\ \vdots \\ v'_n \\ t \end{bmatrix} \le \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Classifying reaction coupling

There are five possibilities

1. $0 \leq \frac{v_i}{v_j} \leq c$ for some constant $c > 0$ **directional coupling $\boldsymbol{i \rightarrow j}$**
2. $c_1 \leq \frac{v_i}{v_j} \leq c_2$ for some constant $c_1 > 0$ and $c_2 > 0, c_1 \neq c_2$ **partial coupling $\boldsymbol{i \leftrightarrow j}$**
3. $\frac{v_i}{v_j} = c$ for some constant $c > 0$ **full coupling $\boldsymbol{i \Leftrightarrow j}$**
4. $c \leq \frac{v_j}{v_i}$ for some constant $c > 0$, without an upper bound **directional coupling $\boldsymbol{i \rightarrow j}$**
5. $0 \leq \frac{v_i}{v_j}$ without an upper bound **uncoupled**

We cannot solve unbounded problems.

The ratio $\frac{v_i}{v_j}$ will be at the upper bound defined from the system!