Positive solutions to linear systems

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Algebraic problem

Let R be a partially ordered ring and let $I \subseteq R[x_1, \dots, x_n]$ be a 0-dimensional ideal.
We want to determie

$$\#V(I) \cap k(R)^n_{\geq 0}$$

Positive real roots of polynomials

Descartes' rule of signs

Let $p(x) \in \mathbb{R}[x]$. The number of **sign changes** between two consecutive nonzero coefficients is an upper bound for the number of positive roots of $p(x)$. Moreover, their difference is an even number.

Positive real roots of polynomials

Sturm's theorem

Let $p(x) \in \mathbb{R}[x]$. Define recursively the so-called Sturm sequence by

$$p_0(x) = p(x), \quad p_1(x) = p'(x), \quad p_{i+1}(x) = -rem(p_{i-1}, p_i) \;\; i \geq 1.$$

The sequence stops when $p_{i+1} = 0$. Let p_m be the last nonzero polynomial.
For $c \in \mathbb{R}$, let $\sigma(c)$ be the number of **sign changes** in the sequence $p_0(c), \dots, p_m(c)$.

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Let $a < b$ and assume that neither a nor b are multiple roots of $p(x)$.

Then $\sigma(a) - \sigma(b)$ is the **number of distinct roots** of $p(x)$ in the interval $(a, b]$.

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Then $\sigma(a) - \sigma(b)$ is the **number of distinct roots** of $p(x)$ in the interval $(a, b]$.

To count positive roots set $a = 0$ and $b = \infty$

Positive real roots of polynomials

Theorem of Kurtz

Let $m \geq 1$ and let

$$p(x) = x^{2m+1} - c_1 x^{2m} + c_2 x^{2m-1} + \cdots + c_{2m} x - c_{2m+1}$$

with $c_i \geq 0$ for all i and let $c_0 = 1$. If

$$c_i^2 - 4c_{i-1}c_{i+1} > 0$$

for all $i = 1, \ldots, 2m$, then $p(x)$ has $\mathbf{2m+1}$ distinct **positive real** roots.

Multivariate polynomials

Multivariate Descartes' rule for (at most) one positive real root

Let $A \in \mathbb{R}^{n \times r}$ and $B \in \mathbb{R}^{r \times n}$ be matrices with full rank. If for all index sets $J \subseteq [r]$ of cardinality n the sign of the products

$$\det(A_{[n],J}) \det(B_{J,[n]})$$

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that are nonzero is always the same, and at least one is nonzero, then there is **at most one postive** solution to

$$Ax^B = y$$

for any $y \in \mathbb{R}^n$.

Multivariate polynomials

Fewnomial bound (Khovanskii)

A system of n real polynomials in n variables involving $1 + \ell + n$ distinct monomials has at most

$$2^{\binom{\ell+n}{2}}(n+1)^{\ell+n}$$

nondegenerate positive solutions.

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Systems supported on circuits (Bihan)

A polynomial system supported on a circuit has at most $n+1$ nondegenerate positive solutions, and this bound is attained.

Circuit: $n+2$ vectors in $\mathbb{Z}^n$ that affinely span $\mathbb{R}^n$

Rational univariate parametrisation

Given a system of complex polynomials with a finite number of solutions, the solutions can be written as

$$\{p_0(T) = 0, x_i = \frac{p_i(T)}{q(T)}, i = 1, \dots, n\}$$

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It is not clear how to study the **positivity** of the different solutions (work in progress)

Particular case: Linear systems

Consider $A \in R^{n \times n}$, $b \in R^n$ and the equations

$$Ax + b = 0$$

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We will associate a **multidigraph** to the system in order to give a different criteria

Graphs

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$$\mathcal{E}_{ji} = \{e \in \mathcal{E} \mid s(e) = j,\ t(e) = i\}$$

The **Laplacian** of $\mathcal{G}$ is the $(m+1) \times (m+1)$ matrix $L = (L_{ij})$ with

$$L_{ij} = \sum_{e \in \mathcal{E}_{ji}} \pi(e) \quad \text{for } i \neq j, \qquad \text{and} \qquad L_{ii} = -\sum_{k \neq i} L_{ki}$$

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The **canonical multidigraph** with Laplacian L is defined as the labeled multidigraph with node set $\mathcal{N} = \{1, \dots, m+1\}$ and one edge $j \to i$ with label L_{ij} for each nonzero entry $L_{ij} \neq 0$, for $i \neq j$

Graphs

Rooted spanning tree: connected subgraph containing all nodes and no cycles with all paths directed towards the root

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Matrix-Tree Theorem

Let L be the Laplacian of $\mathcal{G}$ and $i, j \in \mathcal{N}$
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Then

$$L_{(i,j)} = (-1)^{m+i+j}\ \Upsilon_{\mathcal{G}}(j),$$

where $\Upsilon_{\mathcal{G}}(j)$ is the sum of the labels of all spanning **trees** rooted at j

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$$L = \left(\begin{array}{c|c} A & b \\ \hline \ldots & . \end{array}\right) \text{ with column sums equal to zero}$$

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Proposition

$$\det(A) = (-1)^m \Upsilon_{\mathcal{G}}(m+1)$$

If $\det(A) \neq 0$, then the solution to $Ax + b = 0$ is

$$x_i = \frac{\Upsilon_{\mathcal{G}}(i)}{\Upsilon_{\mathcal{G}}(m+1)} \qquad i = 1, \dots, m$$

Example

$z_1, \ldots, z_5 \in R_{>0}$

$$\begin{pmatrix} -z_2 & 0 & z_4 \\ -z_1 & -z_3 & 0 \\ -z_2 & z_3 & -z_4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} 0 \\ z_5 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

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$$L = \left(\begin{array}{ccc|c} -z_2 & 0 & z_4 & 0 \\ -z_1 & -z_3 & 0 & z_5 \\ -z_2 & z_3 & -z_4 & 0 \\ \hline z_1 + 2z_2 & 0 & 0 & -z_5 \end{array}\right)$$

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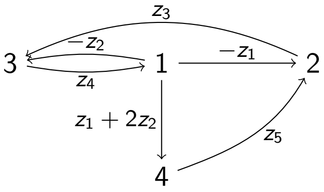

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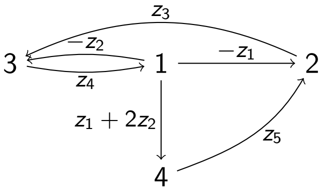

Therefore,

$$\Upsilon_{\mathcal{G}}(2) = (z_1 + 2\,z_2)\,z_4 z_5 - z_1 z_4 z_5 = 2z_2 z_4 z_5$$
$$\Upsilon_{\mathcal{G}}(4) = -\det(A) = (z_1 + 2\,z_2)\,z_3 z_4$$

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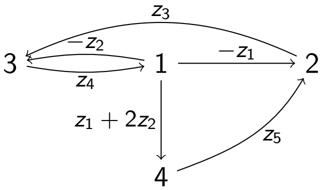

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$$x_1 = \frac{z_5}{z_1 + 2\,z_2} \qquad x_2 = \frac{2\,z_2 z_5}{(z_1 + 2\,z_2)\,z_3} \qquad x_3 = \frac{z_2 z_5}{(z_1 + 2\,z_2)\,z_4}$$

P-graphs

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(i) $\mathcal{E} = \mathcal{E}^{+} \sqcup \mathcal{E}^{-}$

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- (d) $\pi(e) + \sum_{e' \in \mu(e)} \pi(e') \in R_{\geq 0}$

Positivity

Theorem

Let $A \in R^{m \times m}$ with $\det(A) \neq 0$, $b \in R^m$, $x = (x_1, \ldots, x_m)$, and L the associated Laplacian.
If there exists a **P-graph** with Laplacian L, then each component of the solution to the linear system $Ax + b = 0$ is **positive**

Example

$$L = \left(\begin{array}{ccc|c} -z_2 & 0 & z_4 & 0 \\ -z_1 & -z_3 & 0 & z_5 \\ -z_2 & z_3 & -z_4 & 0 \\ \hline z_1 + 2z_2 & 0 & 0 & -z_5 \end{array}\right)$$

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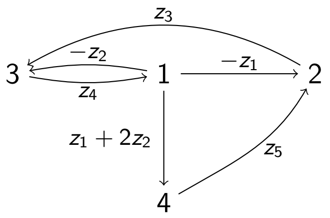

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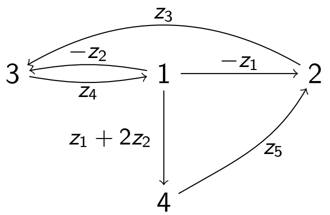

$$\mu(1 \xrightarrow{-z_1} 2) =$$

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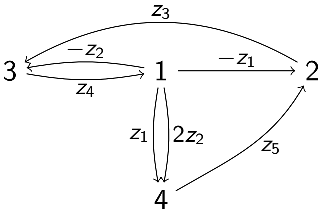

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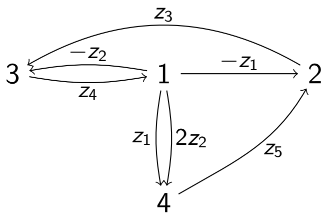

$$\mu(1 \xrightarrow{-z_1} 2) = \{1 \xrightarrow{z_1} 4\}$$

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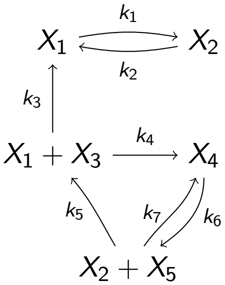
Application: Biochemical reaction networks

Biochemical reaction networks

- $\mathcal{X} = \{X_1, \ldots, X_n\}$ is a finite set of species
  Denote $x = (x_1, \ldots, x_n)$ their concentrations



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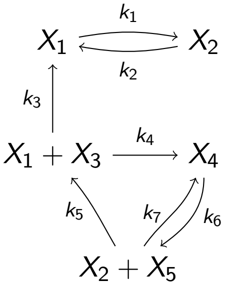

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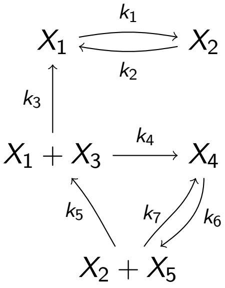
- $(\mathcal{C}, \mathcal{R})$ is a labeled digraph without self-loops
  The edges are defined by a set of reactions $\mathcal{R}$

$$r: \; y_r \xrightarrow{k_r} y'_r, \quad \boldsymbol{k_r} \in \mathbb{R}_{\geq \mathbf{0}}$$



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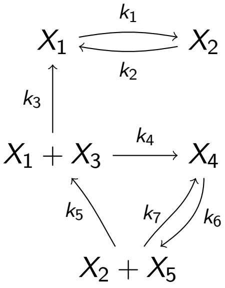

Mass action kinetics: rate function for $r \in \mathcal{R}$:

$$k_r \, x_1^{(y_r)_1} \cdots x_n^{(y_r)_n}$$

Mathematical model

ODE system: $$\dot{x} = \frac{\partial x}{\partial t} = \sum_{r \in \mathcal{R}} (y'_r - y_r) k_r \, x_1^{(y_r)_1} \cdots x_n^{(y_r)_n}$$

Mathematical model

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Stoichiometric subspace: $S = \langle y_r' - y_r \mid r \in \mathcal{R} \rangle \subseteq \mathbb{R}^n$

The stoichiometric compatibility class of $x_0 \in \mathbb{R}^{\boldsymbol{n}}_{\geq \mathbf{0}}$ is

$$P_{x_0} := (x_0 + S) \cap \mathbb{R}^n_{\geq 0} = \{x \in \mathbb{R}^n_{\geq 0} \mid x_0 - x \in S\}$$

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Conservation laws: If $\omega \in S^\perp$ then $\sum_{i=1}^{n} \omega_i \, \dot{x}_i = 0$, so $\omega \cdot x = T$

Steady state equations:

$$\dot{x} = 0 \quad \text{i.e.} \quad 0 = \sum_{r \in \mathcal{R}} (y'_r - y_r) k_r \, x_1^{(y_r)_1} \cdots x_n^{(y_r)_n}$$

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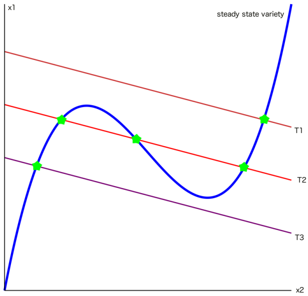
Polynomial system of equations that defines the steady state variety

Steady state variety

The goal is to find a parametrization of the positive part of the steady state variety or its intersection with a stoichiometric compatibility class



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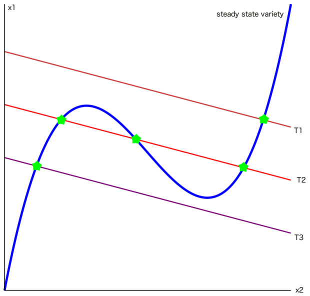

How? Reducing the number of variables in the system by solving the equations iteratively (using linearity)

Reactant-noninteracting sets

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Particular case: noninteracting sets

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Positivity of the elimination

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Definition

Take the graph with node set $\mathcal{U}$ and edge set given, for every $r \in \mathcal{R}$, by the edges

$$X_i \xrightarrow{(r,\ (y'_r)_j)} X_j \quad \text{if } X_i \text{ in the reactant of } r$$
$$\text{and } X_j \text{ in the product of } r$$

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What if one wants to include the conservation laws?

System's structure

$$A = \left(\begin{array}{ccccc} A_1 & 0 & \cdots & 0 & 0 \\ 0 & A_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & A_d & 0 \\ \hline & & A_0 & & \end{array}\right) \in R^{m \times m}, \qquad b = \left(\begin{array}{c} b^1 \\ b^2 \\ \vdots \\ b^d \\ \hline b^0 \end{array}\right) \in R^m$$

with $A_0 \in R^{m_0 \times m}$ and $b^0 \in R^{m_0}$ arbitrary and for $i = 1, \ldots, d$

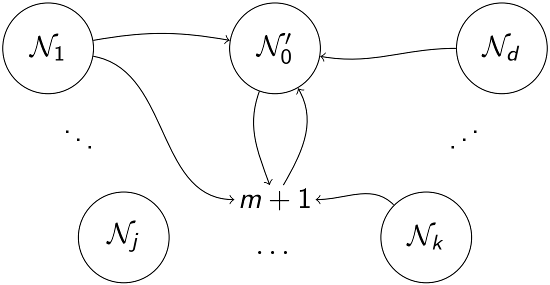
(i) A_i is a square matrix of size m_i

(ii) b^i is a vector of size m_i and nonzero in at most one entry

Graph's structure

Let $\mathcal{G}$ be a labeled multidigraph with $m+1$ nodes and Laplacian L. Then $\mathcal{G}$ is said to be ***A*-compatible** if

(i) There is not an edge from a node in $\mathcal{N}_i$, $i \geq 0$, to a node in $\mathcal{N}_j$ for $i \neq j$, $j \geq 1$



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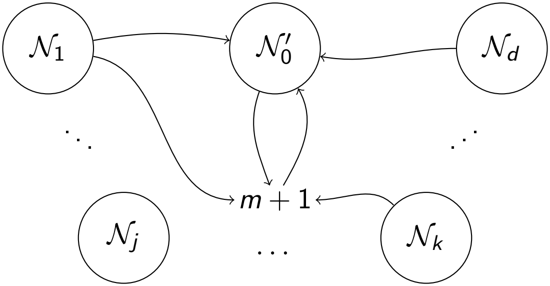
(ii) The ℓ-th row of L agrees with the ℓ-th row of $A|b$ for $\ell \notin \{j_1, \ldots, j_d, m+1\}$



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(*) for $\ell \in \{1, \ldots, m\}$ and $i \in \{1, \ldots, d\}$, any **path** from $j_i \in \mathcal{N}_i$ to ℓ that contains an edge in $\mathcal{E}^-$ goes through $m+1$.

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Then, each component of the solution to $Ax + b = 0$ is **positive**

Elimination system

If $\mathcal{U} \subseteq \mathcal{X}$ let

$$S_{\mathcal{U}}^{\perp} := \{\omega \in S^{\perp} \mid \mathrm{supp}(\omega) \subseteq \mathcal{U}\} \subseteq S^{\perp}$$

conservation laws that relate the species in $\mathcal{U}$ only

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The criteria for positivity applies considering only the species not in the support of $S_{\mathcal{U}}^{\perp}$

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Then the solution to the elimination system is positive

Example

Consider the following reaction network

$$X_1 + U_2 \xrightarrow{k_1} U_1 + U_3 \qquad U_4 \underset{k_3}{\overset{k_2}{\rightleftharpoons}} X_1 \qquad U_1 \xrightarrow{k_4} U_2$$

$$X_1 + U_3 \xrightarrow{k_5} U_4 + U_5 \qquad U_4 \xrightarrow{k_6} U_3 + U_5 \qquad U_5 \underset{k_8}{\overset{k_7}{\rightleftharpoons}} 0$$

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Elimination system: $0 = u_1 + u_2 - T$

$$\begin{aligned} 0 &= -k_4 u_1 + k_1 x_1 u_2, & 0 &= k_1 x_1 u_2 - k_5 x_1 u_3 + k_6 u_4, \\ 0 &= \quad k_5 x_1 u_3 - (k_2 + k_6) u_4 + k_3 x_1, & 0 &= k_5 x_1 u_3 + k_6 u_4 - k_7 u_5 + k_8 \end{aligned}$$

linear in $u_1, \ldots, u_5$

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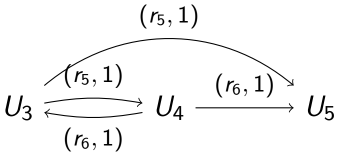

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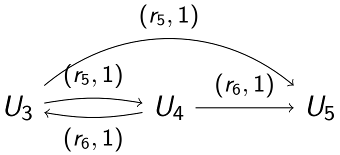

The set $\mathcal{T}$ is

$$\left\{X_1 + U_3 \xrightarrow{k_5} U_4 + U_5, \quad U_4 \xrightarrow{k_6} U_3 + U_5\right\}$$

Example

The solution is

$$u_1 = \frac{Tx_1 k_2}{k_1 x_1 + k_4}$$

$$u_2 = \frac{k_4 T}{k_1 x_1 + k_4}$$

$$u_3 = \frac{k_1 k_3 k_6 x_1 + k_3 k_4 k_6 + (k_2 + k_6) k_1 k_4 T}{k_2 k_5 (k_1 x_1 + k_4)}$$

$$u_4 = \frac{x_1 (k_1 k_3 x_1 + k_3 k_4 + k_1 k_4 T)}{k_2 (k_1 x_1 + k_4)},$$

$$u_5 = \frac{2\, k_1 k_3 k_6 x_1^2 + (2\, k_4 k_3 k_6 + k_1 k_2 k_8 + k_1 k_4 (k_2 + 2\, k_6) T) x_1 + k_2 k_4 k_8}{k_2 k_7 (k_1 x_1 + k_4)}$$

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The conditions for the second case translate into conditions on the reaction network as well

Thank you for your attention

Questions?