

Sparse polynomial systems in chemistry

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Find positive steady states of

$$\dot{x} = f(x), \quad v_i^t x - c_i = 0$$

Maple-Software: storch 1.0

Literatur:

K. Gatermann, B. Huber: JSC 2002

K. Gatermann: Cont. Math. 2001

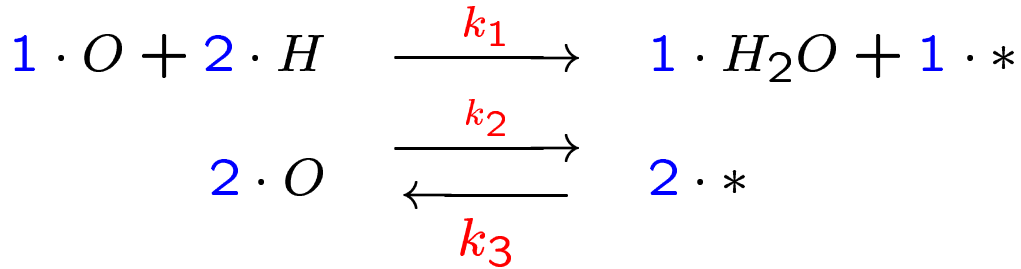
K. Gatermann, M. Wolfrum: preprint 2003

Computeralgebra-Tagung, **Kassel, 15.5. 2003**

Overview

- I. Definition of polynomial system
- II. Version of **Bernstein's 2. Theorem**
- III. **Several positive** solutions

Example



Each arrow gives a column times monomial for

$\dot{X} = f(X)$ in the unknowns $X = (X_o, X_H, X_{H_2O}, X_*)$:

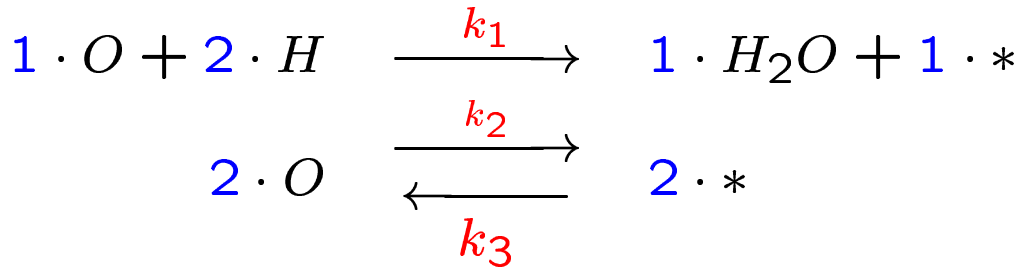
$$\dot{X} = \begin{pmatrix} -1 & -2 & 2 \\ -2 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 2 & -2 \end{pmatrix} \begin{pmatrix} k_1 X_o X_H^2 \\ k_2 X_o^2 \\ k_3 X_*^2 \end{pmatrix} = N v(X) \quad (\text{Clarke form})$$

$$N = \begin{pmatrix} 1 & 0 & 2 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 2 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & 1 & -1 \end{pmatrix} = Y I_a$$

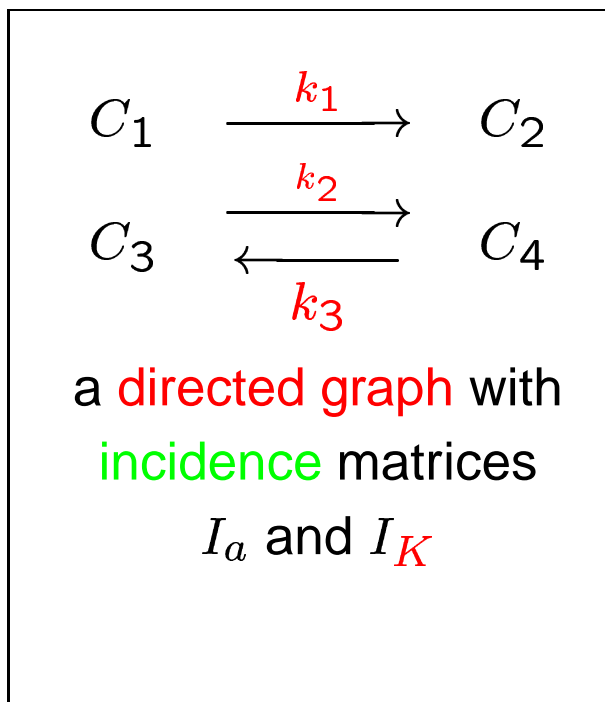
$$v(X) = \begin{pmatrix} k_1 & 0 & 0 & 0 \\ 0 & 0 & k_2 & 0 \\ 0 & 0 & 0 & k_3 \end{pmatrix} \begin{pmatrix} X_o X_H^2 \\ X_{H_2O} X_* \\ X_o^2 \\ X_*^2 \end{pmatrix} = I_K \psi(X)$$

$$\dot{X} = Y I_a I_K \psi(X) \quad (\text{graph-theoretic form})$$

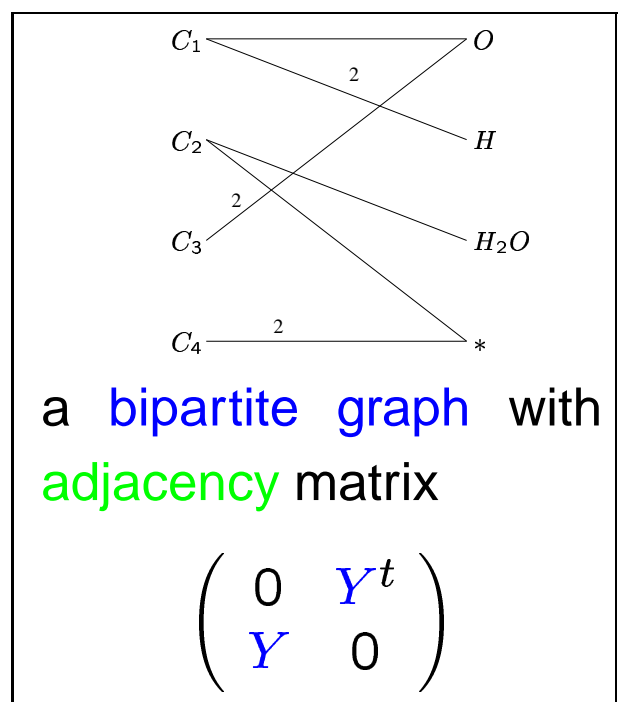
Example



is **equivalent** to



and



The two graphs **define** with $Y = (y_1, \dots, y_4)$

$$\boxed{\dot{x} = Y I_a I_K \psi(x)}, \quad \psi(x) = \begin{pmatrix} x^{y_1} \\ \vdots \\ x^{y_4} \end{pmatrix}$$

Structural analysis of steady states

$$(\dot{x} =) 0 = Y I_a I_K \psi(x) \quad (1)$$

is completed by **linear conservation** relations

$$0 = v_i^t x - c_i, \quad i = 1, \dots \quad (2)$$

(1)+(2) is a family of **sparse** polynomial systems with **special coefficients** depending on parameter k_i, c_i .

Given values of the parameter k_i and c_i

- does a positive solution **exist**?
- is it **unique**?
- are there **several** positive solutions?

Task: Study **all** positive solutions of the **family** (1)

$$\{x \in \mathbb{R}_+^m \mid \exists \underline{k} > 0, Y I_a I_K \psi(x) = 0\}$$

then intersect with (2)

Known results using linear algebra

$$0 = \overbrace{Y I_a}^N \overbrace{I_K \psi(x)}^v = Y \underbrace{I_a I_K}_A \psi(x)$$

I. Clarke's approach: 1980

- compute **positive circuits** of $N = Y I_a$
- results on **dynamics** use **positive circuits**
- **positive circuits** relate to **several** positive solutions

II. Feinberg investigated semi-Laplace matrix $I_a I_K$:

- **deficiency-zero-theorem** and **deficiency-one-theorem** state **unique** positive solutions for special situations
- **deficiency-one-algorithm** states **several** positive solutions for special graphs

Definition: v is called **positive circuit** of N

$:\Leftrightarrow v \geq 0, v \in \ker(N), \text{support}(v)$ is minimal.

Definition: $\text{rank}(I_a) - \text{rank}(Y I_a) = \text{deficiency}$

Alternative coordinates

The **positive solutions** of the family

$$\{x \in \mathbb{R}_+^m \mid \exists \underline{k} \in \mathbb{R}_+^l, \underline{k} > 0, YI_a \underbrace{I_K \psi(x)}_{=z} = 0\}$$

are **mapped** to

$$\begin{aligned} \{[z] \in \mathbb{P}^{l-1} \mid & z \in \ker(YI_a), z > 0, \\ & \exists k_{new} \in \mathbb{R}_+^l, k_{new} > 0, \\ & \text{conditions}(z, k_{new}) = 0\} \end{aligned}$$

Fact: The set $\{z \in \mathbb{R}^l \mid z \in \ker(YI_a), z > 0\}$ is a **convex polyhedral cone** (introduced by Clarke 1981).

We suggest a coordinate **change on parameter**:

$$(k_{new})_j = k_1^{b_{1j}} \cdots k_l^{b_{lj}}, \quad j = 1, \dots, l$$

by a special matrix $B = (b_{ij}) \in GL(l, \mathbb{Z})$

Inverse direction

For $z \in \ker(YI_a)$, $z > 0$ (Clarke's cone) solve $YI_a \underbrace{I_K \psi(x)}_{=z} = 0$ by the **overdetermined** system

$$\begin{array}{rcl}
 z_1 & = & k_1 x_0 x^{y_1} \\
 z_2 & = & k_2 x_0 x^{y_2} \\
 \vdots & & \\
 z_l & = & k_l x_0 x^{y_n}
 \end{array}
 \Leftrightarrow
 \begin{array}{rcl}
 z_1 & = & k_1 x_0 x^{y_1} \\
 \frac{z_2}{z_1} & = & \frac{k_2}{k_1} x^{y_2 - y_1} \\
 \vdots & & \\
 \frac{z_l}{z_1} & = & \frac{k_l}{k_1} x^{y_n - y_1}
 \end{array}$$

if k_i are chosen with $z \in \text{im}(I_K \psi)$ **then**
there **exists** positive solutions

if $\dim(y_2 - y_1, \dots, y_n - y_1) = m$ **then**
there is one **unique** positive solution

else
there is a continuum

Definition (G. '01): (Implicitization of $\text{im}(I_K \psi)$)

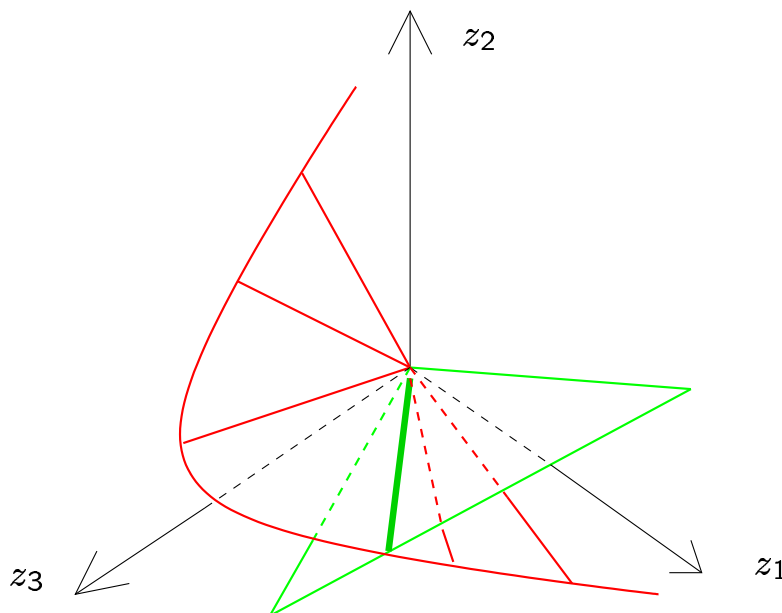
$I_{\hat{Y}}^{def} = \langle \{h(z) \mid h(I_K \psi(x)) \equiv 0, h \text{ homogeneous}\} \rangle$
is called homogeneous **deformed toric ideal**.

$$I_{\hat{Y}}^{def} = \langle z^{g_i^+} - k_{g_i} z^{g_i^-}, \dots \rangle \subset \mathbb{Q}(k)[z]$$

Definition: $\mathbb{Z} \cdot \{y_2 - y_1, \dots, y_n - y_1\}$ is called **lattice**

The algorithm

- compute **generators** of the **cone** $\ker(YI_a) \cap \mathbb{R}_{\geq 0}^l$
- compute **Gröbner basis** of the **deformed toric ideal**
- compute **intersection** z
- solve monomial equations by **Hermite normal form**
- intersect with linear conservation equations



Boundary of Clarke's cone

Question: What happens at the **boundary** of the **convex polyhedral cone** $\ker(Y I_a) \cap \mathbb{R}_{\geq 0}^l$?

There are **two** types of minimal cone generators E_i :

- **cycles** of the directed graph; $I_a E_i = 0$
- **stoichiometric generators**; $I_a E_i \neq 0$

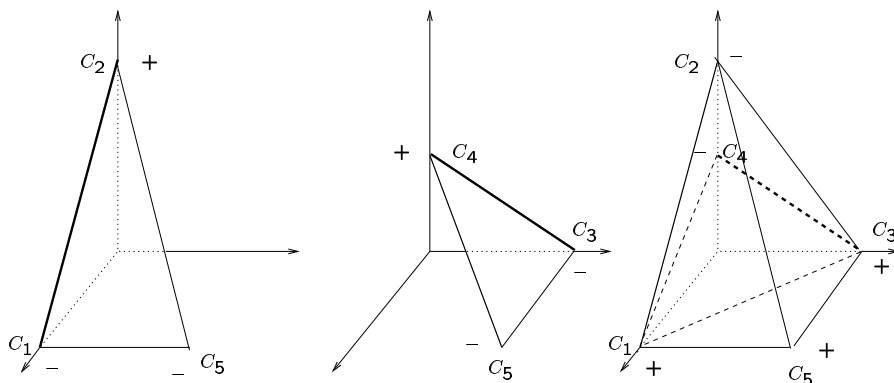
Using Bernstein's 2. Theorem

Definition: The **Newton polytope** of a polynomial $f = c_1 x^{a_1} + \dots + c_m x^{a_m}$ is the convex hull of the exponents a_i .

Def.: A Newton polytope facet defines an **initial facet system** of f_1, \dots, f_n by restriction to the facet.

Theorem: (a) The non-trivial solutions of the **initial facet systems** correspond to solutions at **infinity** or with **zero** components. **(b)** For **mass action** a **cycle** E_i defines a face under mild assumptions and gives rise to non-negative **real** solutions at **infinity** or with **zero** components.

For **mass action** the Newton polytopes are **special**



H_2/O_2 -Example

The generators of the cone include two positive circuits of the directed graph

$$E_1 = [0, 1, 1, 0, 0, 0, 0, 0, 0]$$

$$E_2 = [0, 0, 0, 0, 0, 0, 1, 1, 0]$$

E_1, E_2 each give an edge of the Newton polytope

Result: E_1 corresponds to $x = 0$

E_2 corresponds to the point at infinity

$$\left[0 : 1 : 0 : 0 : 0 : \sqrt{\frac{k_{7,10}}{k_{10,7}}} \right] \in \mathbb{P}^5$$

The deformed toric ideal in this example is

$$I_{\hat{Y}_r}^{def} = \langle k_{5,4}z_4 - k_{9,4}z_5, k_{11,8}^2z_2z_6 - k_{9,3}k_{10,6}z_9^2, \\ k_{9,3}^2k_{10,7}k_{7,10}z_1^2z_3^2 - k_{2,1}^2k_{3,9}^2z_2^2z_7z_8 \rangle$$

Complex balancing solutions

Horn, Jackson '72

Definition: A solution $x > 0$ of $YI_a I_K \Psi(x) = 0$ is called **complex balancing** if $I_a I_K \Psi(x) = 0$

Definition: $g_i = I_a E_i$ is called **confluent vector** for a cone generator E_i .

The g_i suggests a choice of new parameter k_{g_i} .

Lemma: For $k_{g_i} = 1$ each affine space $\{v_i^t x - c_i\}$ has **exactly one** solution which is **complex balancing**.

Proof: After linear algebra there are polynomials with monomials from one connected component each. With the **Cayley trick** we use the multi-homogeneous ideal

$$I_{\widehat{Y}}^{def} = \langle z^{g_i^+} - k_{g_i} z^{g_i^-}, i = 1, \dots, s \rangle : z^\infty$$

given by the **confluent** vectors g_i .

Toric Deformation

Question: For which values of the parameter k_{new} do **several** positive solutions within $\{v_i^t x - c_i = 0\}$ exist?

New Idea: For some linear independent **confluent** vectors g_i consider the **limit**

$$k g_i \rightarrow 0, \quad i = 1, \dots, s$$

Inspiration, application of known theory:

- **Viro method** with artificial parameter $t \rightarrow 0$:
 - Polynomial system breaks into **small subsystems**.
 - By **continuation** solutions of subsystem determine solutions for $t \sim \epsilon$.
- Toric variety deforms into several projective spaces
- Each **reduced Gröbner basis** of toric ideal gives a **regular triangulation** of the Newton polytope

Literatur: GKZ, Sturmfels '96

Multistationarity

$$g_i = I_a E_i$$

Approach: study limit $k_{g_i} \rightarrow 0, i = 1, \dots, s$

- Multihomogeneous toric ideal deforms to leading monomial ideal
- giving a **regular triangulation** of Cayley-graph-polytope
- assume $\text{supp}(g_i^-)$ defines **inner face**
- inner face defines small subsystem
- real solutions of **inner face system known** from E_i
- $k_{g_i} = 0$ corresponds to some $k_j = 0$
- means dropping of vertices of polytope
- Positive solutions coming from **infinity**

Cone generators E_i are **source** of multistationarity.

Result: **Several** positive solutions are expected in the parameter region with $k_{g_i} \simeq \varepsilon$.

Inner face subsystems

A stoichiometric cone generator E_i defines a special **subsystem** by its support.

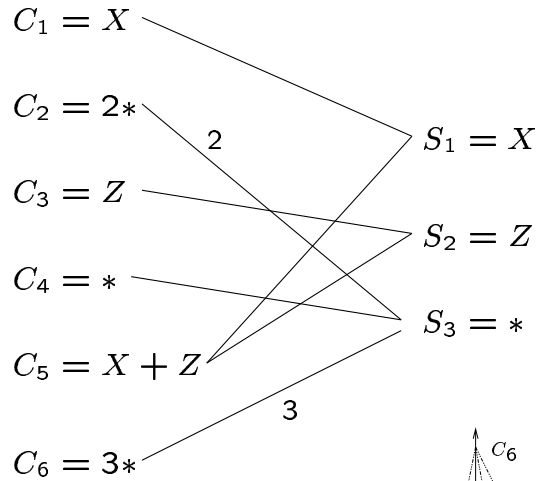
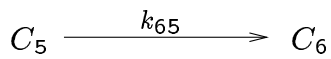
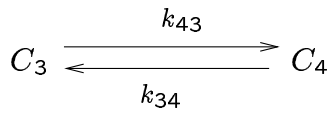
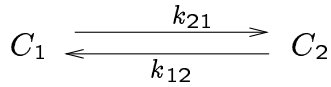
Proposition: Assume

- (i) the directed graph is a **forest of trees**
- (ii) there is one stoichiometric generator
- (iii) \widehat{Y}_r has maximal rank
- (iv) exists $\mu \in \text{span}(y_2 - y_1, \dots, y_r - y_1)^\perp$,
not orthogonal to $\text{im}(Y I_a)$

Then for some $c_i > c_i^*$ there are **two** solutions of

$$Y I_a I_K \Psi(x) = 0, \quad v_i^t x - c_i = 0$$

Example

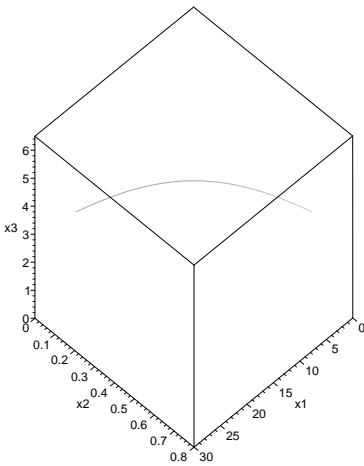
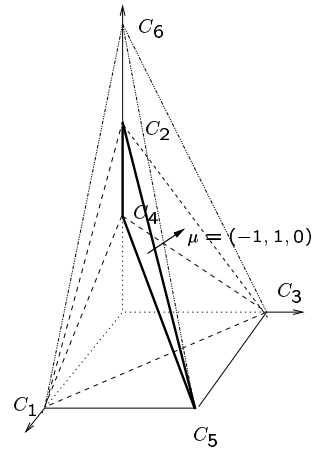


$$E_3 = (0, 1, 0, 1, 1)$$

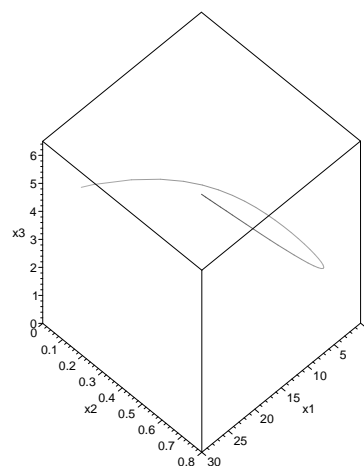
$$g_3 = (1, -1, 1, -1, -1, 1)$$

$$k_{g_3} = k_{21}k_{43}/(k_{12}k_{34}k_{65}) \rightarrow 0$$

yields regular triangulation of the Newton polytope with **inner face**



solutions of **subsystem**



solution curve