Bernstein’s second theorem and Viro’s method for sparse polynomial systems in chemistry

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Abstract
We consider a family of sparse polynomial systems defined by a directed graph and a bipartite graph which depend on certain parameters. A convex polyhedral cone serves as a representative of all positive solutions of the family. We study the boundary of this cone with Bernstein’s second theorem and Viro’s method. In particular we present new results about the parameter regions where several positive solutions appear. Since they are steady states of an underlying dynamical system of mass action kinetics, the resulting multistationarity has important implications for the dynamics of that system. Examples from applications illustrate the theoretical results.

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1. Introduction
We consider a family of sparse (Laurent) polynomial systems of the form

\[ 0 = Y_{\text{I}} I_{\text{K}} \Psi(x), \quad \Psi_j(x) = x^{\eta_j}, \quad j = 1, \ldots, n, \quad (1) \]
\[ 0 = v_i^T x - c_i, \quad i = 1, \ldots, r, \quad (2) \]

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where $Y_s$ is a fixed matrix in $(\mathbb{Z}_{\geq 0})^{m,n}$, the set of $(m \times n)$-matrices with non-negative integer entries, $I_a$ a fixed matrix in $\mathbb{Z}^{n,t}$, $n_j$ is a fixed vector in $\mathbb{Z}^m$, $v_i$ is a fixed vector in $\mathbb{R}^m$. $I_K$ is a matrix in $(\mathbb{Q}[k])^{n,m}$, where $\mathbb{Q}[k]$ is the ring of polynomials in the parameters $k_{ij}$ (which can take positive real values), and $c_i$ are real constants. In particular, the polynomial system depends on the parameters $k_{ij}$ and the constants $c_i$. These systems arise when studying the steady states of a differential system, modeling chemical reactions with mass action kinetics. The linear equations (2) are conservation relations, like, e.g., conservation of mass. There are many results about such systems in the literature in chemistry and applied mathematics, including [6,15,16,18,24,26,30,36].

For fixed values of the parameters $k_{ij}$ the set of all positive solutions of (1) is mapped onto $\{[z_1 : z_2 : \cdots : z_t] \in \mathbb{P}^{t-1} \mid z \in \ker(Y_s I_a) \cap \mathbb{R}^t, p_i(z; k) = 0, i = 1, \ldots, t\}$, where $p_i = z^\alpha_i - \gamma_i(\vec{k})z^\eta_i \in \mathbb{R}[z]$ are special homogeneous polynomials. The simple reason is that for a positive solution $x$ the vector $z = I_K \Psi(x)$ is positive and in the nullspace of $Y_s I_a$. The set $\ker(Y_s I_a) \cap (\mathbb{R}^{\geq 0})^t$ is a convex polyhedral cone. On the other hand $z$ is in the image of $(\mathbb{R} \setminus \{0\})^n \to \mathbb{R}^t, x \mapsto I_K \Psi(x)$. The image is described implicitly by an ideal $I = \langle g_1, \ldots, g_l \rangle \subseteq \mathbb{R}[z]$ analogous to a toric ideal. The variety $V(I) \subseteq \mathbb{P}^{t-1}$ is the Zariski closure of $\text{im}(I_K \Psi)$. It is the Zariski closure of the maximal orbit $O_{I_K 1}$ of a torus action induced by the monomials $x^\eta_i$.

For each positive $z$ in the cone $\ker(Y_s I_a) \cap (\mathbb{R}^{\geq 0})^t$, there exists positive values of $k_{ij}$ such that $z \in \text{im}(I_K \Psi)$ and consequently $p_i(z; k) = 0, i = 1, \ldots, t$. The set of all positive solutions of the family $\{x \in \mathbb{R}^t \mid \exists k_{ij} > 0 \text{ with } Y_s I_a I_K \Psi(x) = 0\}$ is mapped onto $\{[z_1 : z_2 : \cdots : z_t] \in \mathbb{P}^{t-1} \mid z \in \ker(Y_s I_a) \cap \mathbb{R}^t\}$. Thus the interior of the convex polyhedral cone represents all positive solutions of the family. For arbitrary parameters $k_{ij} > 0$, we view $p_i = z^\alpha_i - \gamma_i(\vec{k})z^\eta_i$ as elements in $\mathbb{Q}(\vec{k})[z]$. In [21] we called $I = \langle g_1, \ldots, g_l \rangle \subseteq \mathbb{Q}(\vec{k})[z]$ a deformed toric ideal. Background on toric geometry can be found in [7,14,19,34]. Instead of abstract toric varieties, we are using the language of embeddings of toric varieties which is more appropriate for applications.

The minimal generators of the cone $\ker(Y_s I_a) \cap (\mathbb{R}^{\geq 0})^t$ are fundamental to the analysis of stability of steady states and the occurrence of Hopf bifurcation in [6], see also [10–12]. This is the reason why we answer the following questions in the paper: How does the boundary of the cone relate to non-negative real solutions of the family (1)? Which values of the parameters $k_{ij}$ are relevant for this?

The main insight is that there are two different types of minimal generators of the cone. The first type are positive circuits $E_i$ of a directed graph with $I_a E_i = 0$, the second type are the so-called stoichiometric generators ($I_a E_i \neq 0$).

In this paper we relate the positive circuits of the directed graph to Bernstein’s second theorem [2,5,9,25]. This theorem is relating solutions at infinity or with zero-components to the facets of the Newton polytopes. A subsystem defined by a positive circuit equals under mild conditions an initial face system. The simple reason is that only a few chemical species are involved in each reaction or, equivalently, the monomials have sparse support. Thus a positive circuit gives asymptotic information about steady states for extreme values of mass.

Systems whose cone $\ker(Y_s I_a) \cap (\mathbb{R}^{\geq 0})^t$ is generated by positive circuits have the property that each affine space $\{x \in \mathbb{R}^m \mid v_i^T x - c_i = 0\}$ contains a unique positive solution.
Thus stoichiometric generators are a source for several positive solutions (multistationarity). This is explained by generalizing Viro’s method \[9,22,32,33,35\] for the study of the number of positive solutions. We replace the role of the monomials \(\Psi_j(x) = x^{\eta_j}\) in the standard theory by \((I_K \Psi(x))_i = k_{ij}x^{\eta_i}\). We replace the artificial parameter in the classical method by the parameters \(k_{gi} = k_i^g\), where \(g_i = L_iE_i\). An important ingredient are Stanley–Reisner ideals of regular triangulations of the Cayley-graph-polytope. Our main theorem is Theorem 4.18. Multistationarity has important implications for the dynamics of the underlying differential equation, e.g., in the context of singular perturbation theory or for the existence of reaction–diffusion waves.

2. Sparse polynomials from mass action kinetics

First we introduce the equations as presented in \[20,21\], being slightly more general so as to allow Laurent polynomials. Then, we outline the main principle, along with some computational issues.

2.1. Sparse equations on graphs

A system of chemical reactions with chemical species \(S_1, \ldots, S_m\) is given as

\[
\begin{align*}
a_{11}S_1 + \cdots + a_{m1}S_m & \xrightarrow{k_1} b_{11}S_1 + \cdots + b_{m1}S_m, \\
a_{12}S_1 + \cdots + a_{m2}S_m & \xrightarrow{k_2} b_{12}S_1 + \cdots + b_{m2}S_m, \\
& \vdots \\
a_{1l}S_1 + \cdots + a_{ml}S_m & \xrightarrow{k_l} b_{1l}S_1 + \cdots + b_{ml}S_m
\end{align*}
\]

with given \(A = (a_{ij}), B = (b_{ij}) \in (\mathbb{Z}_{\geq 0})^{m \times l}\), and real numbers \(k_i > 0, i = 1, \ldots, l\), called rate constants. Then a polynomial system is defined. For each reaction a vector is formed by the differences of the coefficients on the right and the left and is multiplied with the monomial \(\vec{v}_i = k_i \prod_{j=1}^{m} x_j^{a_{ij}}\). With \(N = B - A\)

\[
0 = (B - A) \begin{pmatrix} k_1x_1^{a_{11}} & \cdots & x_m^{a_{1m}} \\
\vdots & \ddots & \vdots \\
k_1x_1^{a_{l1}} & \cdots & x_m^{a_{lm}} \end{pmatrix} = N\vec{v}(x).
\]

These are the equations for the steady states of the corresponding mass action kinetics. Sometimes the exponents differ slightly from \(a_{ij}\). Such systems are then called generalized mass action kinetics.

Example 2.1. The reaction laws in Fig. 1 describe the oxidation of \(H_2\) on a catalytic surface \[10,20\]. There are \(m = 5\) species, and \(l = 9\) reactions. \(x_1, \ldots, x_5\) are the concentrations of \(O, H, H_2O, H_2O_f\) and the amount of free space on the surface, respectively. The equations for the steady states of generalized mass action kinetics are here
For the last reaction, the monomial $x_2 x_4$ instead of $x_2^2 x_4^2$ has to be used as indicated by underbracing. Presenting the equations in this form has some obvious drawbacks. For example the second and third column are the same except of the sign. The monomial $x_3$ appears twice with different rate constants. The system will be rewritten below.

Some of the left-hand sides and right-hand sides of the reactions (3) may be equal. We refer to them as complexes $C_j$, $j = 1, \ldots, n$. On this level of abstraction, (3) is a directed graph with vertices $C_j$, $j = 1, \ldots, m$, and oriented edges (arrows) $C_j \rightarrow C_i$ with weights $k_{ij} > 0$. Here, $C_j$ is called reactant complex or educt complex, while $C_i$ is called product complex. This directed graph has two incidence matrices. The first incidence matrix is $I_a = (w_{ij})_{i=1,\ldots,n,j=1,\ldots,l}$, where $w_{ij} \in \{-1, 0, 1\}$ and $l$ denotes the number of arrows. Each column represents an oriented edge by containing one entry $-1$ for the reactant and 1 for the product. The second incidence matrix is $I_K = (u_{\mu\nu})_{\mu=1,\ldots,l;\nu=1,\ldots,n}$ with $u_{\mu\nu} \in \{k_{ij} \mid i, j = 1, \ldots, n\}$, or $u_{\mu\nu} = 0$. Each row corresponds to one oriented edge and has at most one non-zero entry. The $\mu$th arrow $C_j \rightarrow C_i$ gives $u_{\mu j} = k_{ij}$ encoding the weight and that $C_j$ is the initial vertex.

We still need the information that each complex $C_j$ is a linear combination $\sum_{i=1}^{m} y_{ij} S_i$ of species $S_i$ with coefficients $y_{ij} \in \mathbb{Z}_{\geq 0}$. This is given by a weighted bipartite graph. The two sets of vertices consist of chemical species $S_i$, $i = 1, \ldots, m$, and complexes $C_j$. 

\[
0 = \begin{bmatrix}
-1 & 0 & 0 & 0 & 0 & -2 & 2 & 0 \\
-2 & -2 & 2 & 0 & 0 & 0 & 0 & -2 \\
1 & 0 & 0 & -1 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & -2 & 0 & 0 \\
1 & 1 & -1 & 1 & 0 & 2 & 2 & -2 \\
\end{bmatrix}
\begin{bmatrix}
k_{2,1} x_1 x_2^2 \\
k_{9,3} x_2^2 \\
k_{9,5} x_5 \\
k_{9,4} x_3 \\
k_{5,4} x_3 \\
k_{10,6} x_4^2 \\
k_{10,7} x_5^4 \\
k_{7,10} x_3^2 \\
k_{11,8} x_2 x_4 \\
\end{bmatrix}
\]
For each edge \( \{S_i C_j\} \) there is a weight \( y_{ij} \in \mathbb{Z}_{\geq 0} \). This defines the weighted adjacency matrix

\[
\begin{pmatrix}
0 & Y_s \\
Y_s' & 0
\end{pmatrix},
\]

with \( Y_s = (y_{ij})_{i=1,\ldots,m, j=i,\ldots,n} \). We denote the columns of \( Y_s \) by \( y_1, \ldots, y_n \in (\mathbb{Z}_{\geq 0})^m \). Then \( N = Y_s I_a \) since \( I_a \) contains exactly one \(-1\) and one \(1\) in each column. This means differences of columns of \( Y_s \) are formed. But the columns of \( Y_s \) contain the coefficients of complexes in (3). Defining \( \Psi_j(x) = x^{y_j}, \ j = 1, \ldots, n \), we have \( \tilde{v}(x) = I_K \Psi(x) \).

For a generalized mass action system the exponents differ from \( y_{ij} \) in some places. This can be incorporated in this model by choosing a second set of weights \( \eta_{ij} \) on the edges of the bipartite graph. This defines a second weighted adjacency matrix with block \( Y_k \in \mathbb{Z}^{m,n} \).

We denote the columns of \( Y_k \) by \( \eta_1, \ldots, \eta_n \in \mathbb{Z}^m \) and use \( \Psi_j(x) = x^{\eta_j}, \ j = 1, \ldots, n \).

Altogether, this leads to the following Laurent polynomial equations

\[
0 = Y_s I_a I_K \Psi(x), \quad \text{with} \quad \Psi(x) = \begin{pmatrix} x^{\eta_1} \\ \vdots \\ x^{\eta_n} \end{pmatrix}.
\]

We are interested in positive (or at least non-negative) solutions.

**Remark 2.2.** In this application, we can state some obvious restrictions on the graphs. For the weighted directed graph we assume that for each vertex \( C_i \) there is at least one incident edge. An oriented edge \( C_j \rightarrow C_i \) and its opposite \( C_i \rightarrow C_j \) with two associated constants \( k_{ij} \) and \( k_{ji} \) are simultaneously possible. They are called reversible reactions. But there are no parallel edges. For the bipartite graph, we assume that \( Y_s \) and \( Y_k \) have the same support (i.e., \( y_{ij} = 0 \) iff \( \eta_{ij} = 0 \)) and that \( \eta_{ij} \leq y_{ij} \), \( \forall i = 1, \ldots, m, j = 1, \ldots, n \). Moreover, we assume that \( y_i \neq y_j \) or \( \eta_i \neq \eta_j \) for all \( i \neq j \). Additionally, we assume that every vertex \( S_i \) is adjacent to at least one vertex \( C_j \). But there may be \( C_j \) without incident edges.

System (5) describes the steady state solutions of a dynamical system. This has flow-invariant subspaces of the form \( (x_0 + \text{im}(Y_s I_a I_K)) \cap (\mathbb{R}_{\geq 0})^m \), see [26] or Lemma 2.1 in [21]. Thus linear restrictions

\[
v_i' x - c_i = 0,
\]

\( i = 1, \ldots, m - \text{rank}(Y_s I_a I_K) \), are satisfied in addition. Here, the \( v_i \) form an orthonormal basis of the orthogonal complement of \( \text{im}(Y_s I_a I_K) \) and the \( c_i \in \mathbb{R} \) are given constants. Physically, the meaning is conservation of mass, or moiety, or other quantities.

**Example 2.1 (continued).** The weighted directed graph and weighted bipartite graph of this example are presented in Fig. 2. There are \( n = 11 \) complexes and
Fig. 2. Weighted directed graph and weighted bipartite graph, describing the chemical reaction from Example 2.1. An edge in the bipartite graph without number has weights $y_{ij} = \eta_{ij} = 1$. If only one number is associated to the edge, then $y_{ij} = \eta_{ij}$, else $y_{ij} > \eta_{ij}$.

$$Y_S = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 & 0 & 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 \end{bmatrix},$$

$$\Psi(x) = (x_1 x_2^2, x_3 x_5, x_2^2, x_3, x_4, x_2^2, x_3, x_2, x_4, x_5, x_2^2, x_5, x_3^2)^T.$$

The equations for the steady states are

\begin{align*}
0 &= -k_{2,1} x_1 x_2^2 - 2k_{10,7} x_1^2 + k_{7,10} x_5^2, \\
0 &= -2k_{2,1} x_1 x_2^2 - 2k_{9,3} x_2^2 - 2k_{11,8} x_2 x_4 + 2k_{3,9} x_5, \\
0 &= k_{2,1} x_1 x_2^2 + ( -k_{5,4} - k_{9,4} ) x_3, \\
0 &= k_{5,4} x_3 - 2k_{10,6} x_4^2 - 2k_{11,8} x_2 x_4, \\
0 &= k_{2,1} x_1 x_2^2 + k_{9,3} x_2^2 + k_{9,4} x_3 + 2k_{10,6} x_4^2 + 2k_{10,7} x_1^2 + 3k_{11,8} x_2 x_4 - k_{3,9} x_5 - 2k_{7,10} x_5^2,
\end{align*}

where the constants $k_{ij}$ are positive real numbers which serve as parameters.

We have $\text{rank}(Y_S I_a I_K) = \text{rank}(Y_S I_a) = 4 < 5 = m$. The additional linear restriction is given by

$$v_1^T x - c_1 = (2 \ 1 \ 2 \ 2) x - c_1 = 0.$$
Remark 2.3. (i) There are equivalent ways of presenting the discrete information of the two graphs. In the chemical literature [6] usually a diagram is drawn. In [36] another graph is introduced. (ii) Also the equations for the steady states can be given in a different form than (4) or (5). For example they can be seen as linear combinations of binomials and monomials.

In the following we will need some matrices $Y_r$, $Y_L$, $Y_e$, whose columns consists of some columns $\eta_j$ of $Y_k$. Some monomials $x^{\eta_j}$ which correspond to pure product complexes $C_j$ do not appear in Eqs. (5), since the corresponding column of $I_K$ is zero. We collect the columns $\eta_j$ whose complexes $C_j$ appear as reactant complexes into the matrix $Y_r$. We assume that we have chosen the numbering such that $Y_r = (\eta_1, \ldots, \eta_r)$. Some complexes appear as reactant complexes several times. So we list these columns of $Y_r$ several times and denote the matrix by $Y_L$. Then $Y_L$ has as columns exactly the exponents of $\vec{v}$ in (4). If we add to $Y_L$ the columns $\eta_j$ of pure product complexes, we denote the new matrix by $Y_e$.

The graph-theoretical interpretation of $Y_r$ is that the bipartite graph is reduced by removing vertices $C_j$ being pure product complexes and their incident edges. For $Y_L$ this bipartite graph is modified by copying the complexes $C_j$ which appear as reactant complexes according to their multiplicity.

2.2. The approach

In [20] the intersection of a deformed toric variety with a convex polyhedral cone has been introduced as a modification of a general principle from toric geometry.

The convex polyhedral cone $\text{ker}(Y_sI_a) \cap (\mathbb{R}_{\geq 0})^l$ has been introduced and studied by B. Clarke [6]. Each ray $[z_1 : \cdots : z_l]$, $z > 0$, in the cone corresponds to some positive solution of (5) for some value of the parameters $k_{ij}$. Such a positive solution $x$ is found as a solution of $z = x_0I_K\Psi(x)$, where we introduced $x_0$ to compensate the ambiguous length of $z$. Thus the interior of the convex polyhedral cone corresponds to all positive solutions of system (5) for any value of the parameters $k_{ij}$.

For fixed values of $k_{ij}$ and given $z > 0$ the system $z = x_0I_K\Psi(x)$ does not have a solution in general. Conditions on $z$ need to be satisfied.

Definition 2.4 [20]. The ideal

$\tilde{I}_{Y_L}^{\text{def}} = \{ f \in Q(\mathbb{C})[z] | f(x_0I_K\Psi(x)) = 0, \forall x_0 \in \mathbb{C}, x \in (\mathbb{C}\setminus\{0\})^m \}$

is called deformed homogeneous toric ideal.

For each choice of positive real $k_{ij}$, the deformed toric ideal reduces to a homogeneous ideal in $\mathbb{R}[z]$. In this special case, we call the associated variety $V(\tilde{I}_{Y_L}^{\text{def}}) \subseteq \mathbb{P}^{l-1}$ deformed projective toric variety. Different choices of values for $k_{ij}$ give a parameterization of the family of projective varieties.

The names deformed homogeneous toric ideal and deformed projective toric variety are justified by the close relation to the homogeneous toric ideal $I_{Y_k} = \{ f \in Q[w] | f(x_0w^n, \ldots, x_0w^m) = 0, \forall x, x_0 \}$. The torus action of the algebraic torus $T = (\mathbb{C}\setminus\{0\})^m$
on $\mathbb{C}^m$ by $x \mapsto (t_1 x_1, \ldots, t_m x_m)$ induces a torus action on $\mathbb{C}^m$ by the matrix $Y_r$. For fixed $k$, the evaluation at $e = (1, \ldots, 1)$ gives $I_k \Psi(e)$. The point generates an orbit $O_k \Psi(e)$ under the torus action. $V(I_{\text{def}})$ is the Zariski closure of this orbit in the projective space. Thus $I_{\text{def}}$ is a prime ideal in $Q(k \mathbb{C})[z]$, which also follows from Corollary 2.6 in [13].

The family of deformed projective toric varieties covers the cone

$$\{[z_1 : \cdots : z_l] \in \mathbb{P}^{l-1} \mid z > 0, \ z \in \ker(Y_s I_a)\}.$$ 

That means for each ray $[z]$ in the interior of the cone there are values of $k_{ij}$ such that $[z] \in V(I_{\text{def}})$. For $[z] \in (I_{\text{def}})$ the system $z = x_0 I_K \Psi(x)$ has at least one positive solution $x \in (\mathbb{R}_+)^m$.

The efficient computation of a Gröbner basis of $I_{\text{def}}$ is done in the following way. Since a vertex $C_j$ may be the initial vertex for several arrows (reactions), there will be linear equations in $I_{\text{def}}$. For example, if the $\mu$th arrow is $C_j \rightarrow C_i$, and the $\nu$th arrow is $C_j \rightarrow C_s$, then $k_{ij} z_\nu - k_{\mu j} z_\mu \in I_{\text{def}}$. Remember from Section 2.1 that $Y_r = (\eta_1, \ldots, \eta_r)$ denotes the matrix of reactant complexes. A Gröbner basis of $I_{\text{def}} = \{ f \in Q[w] \mid f(x^{0 x^D}, \ldots, x^{0 x^D}) = 0, \ \forall x, x\} \text{ is computed. Implementations of special efficient algorithms are available for ex- ample in “Singular” [23]. Some of these algorithms are described in [34, Chapter 12]. In particular, } w^g \quad - w^\gamma \in I_{def} \text{ corresponds to } g = g^\lambda - g^\gamma \in \ker(Y_r). \text{ The columns of } Y_{\text{def}} \text{ are the columns of } Y_r, \text{ but some are repeated. Thus reordering of } g \text{ and filling up with zeros gives } g \in \ker(Y_{\text{def}}). \text{ This way, the Gröbner basis of } I_{\text{def}} \text{ is converted into polynomials in } I_{\text{def}} \text{ using } z = I_K w. \text{ Together with the linear polynomials, this gives the desired Gröbner basis of } I_{\text{def}} \text{ of } Y_{\text{def}}.$$

The cone $\ker(Y_s I_a) \cap (\mathbb{R}_+)^l$ has been investigated a lot by chemists and they implemented algorithms for the computation of a set of minimal generators (see, for example, [29] or [26, Chapter 3] and references therein). Also algorithms from computational geometry [1] are applicable. Intersecting a convex polyhedral cone with a generic hyperplane defines a polytope, whose vertices are enumerated in [1] using the Simplex algorithm and an associated tree. In contrast, the structure of the matrix $Y_s I_a$ is exploited in [29]. The basic idea is that this cone is the smallest cone in a nested chain of cones.

As pointed out in [20], there are two different types of minimal generators of the convex polyhedral cone $\ker(Y_s I_a) \cap (\mathbb{R}_+)^l$. Since $\ker(I_a) \subseteq \ker(Y_s I_a)$, we have also for the cones

$$\ker(I_a) \cap (\mathbb{R}_+)^l \subseteq \ker(Y_s I_a) \cap (\mathbb{R}_+)^l.$$ 

Since $I_a$ is an incidence matrix of a directed graph, minimal generators of $\ker(I_a) \cap (\mathbb{R}_+)^l$ are positive circuits (oriented cycles) of the directed graph. In many cases these positive circuits are also minimal generators of the cone $\ker(Y_s I_a) \cap (\mathbb{R}_+)^l$. For chemical reaction systems, in many cases positive circuits occur as pairs of forward–backward reactions.

**Definition 2.5.** A minimal generator of the convex polyhedral cone $\ker(Y_s I_a) \cap (\mathbb{R}_+)^l$, which is not a positive circuit of the directed graph, is called stoichiometric generator.
The positive circuits are given by the structure of the directed graph. But also the existence of stoichiometric generators is influenced by the directed graph. Besides oriented cycles of the directed graph, we also need the notion of connected component, which is a minimal set of vertices which are connected by paths, and strong connected component, which is a minimal set of vertices such that each pair of vertices lies on an oriented cycle. A terminal strong connected component is a strong connected component with the property that no arrow is pointing out.

These notions are fundamental in the work by Feinberg and others [15,24,30]. They investigate the matrix $I_a I_K$ which is similar to a Laplacian matrix (see [4, p. 27]) and thus has similar properties as shown in [18], see also [21].

By a support of a vector one usually means the components being unequal zero. For a vector in the kernel of $Y_s I_a$, we need a modified definition. Given a vector $v \in \mathbb{C}^l$ by

$$S_v = \{ j \in \{1, \ldots, n\} \mid \exists \mu \in \{1, \ldots, l\} \text{ with } (I_K e_j)_{j\mu} \neq 0 \text{ and } v_{\mu} \neq 0 \},$$

we define the set of indices of initial vertices of arrows (reactant complexes) in the directed graph, to form the support of $v$.

**Lemma 2.6.** Assume there exists a stoichiometric generator $E_i$ such that the support $S_{E_i}$ is contained in strong connected components. For each connected component, let one of the two conditions is satisfied. Either $S_v$ contains at most one entry in this connected component, or the positive circuits are forward–backward reactions. Then there is another stoichiometric generator which depends linearly on $E_i$ modulo positive circuits of the directed graph.

**Proof.** For each non-zero entry in $-E_i$, there is a positive circuit having a positive entry at this position. Thus, a linear combination results in a new stoichiometric generator. □

Please observe that the first assumptions are satisfied, if the directed graph has only connected components which are strongly connected and $\text{rank}(Y_s I_a) < \text{rank}(I_a)$.

The aim of this paper is to clarify the role of these two types of generators. The stoichiometric generators are investigated in Section 4. In Section 3, we relate the positive circuits to the existence of solutions in the limit with zero-components or at infinity. These are projective solutions of certain subsystems of the polynomial system (5).

**Definition 2.7.** For a subgraph of the directed graph, we define a subgraph subsystem by deleting the columns of $I_a$, which do not correspond to arrows in the subgraph, and deleting rows in $I_K$ giving a reduced system $Y_s I_a I_K \Psi(x) = 0$. If the subgraph is a positive circuit, then we call it circuit subsystem. If the subgraph is given by a stoichiometric generator, then we call it stoichiometric subgraph system.

The next section deals with circuit subsystems.
3. Real solutions at infinity

In this section, we derive results for the chemical reaction system (5) which are analogous to Bernstein’s second theorem for general systems of sparse Laurent polynomials (see [2] and Theorem 6.1 in the appendix of [25]). We start by recalling the theory.

3.1. Bernstein’s second theorem

We consider the sparse polynomials

\[ f_i(x) = \sum_{j=1}^{n} c_{ij} x^{a_j}, \quad i = 1, \ldots, r, \]  

where \( c_{ij} \in \mathbb{C} \backslash \{0\} \) are given constants. The exponents \( a_1, \ldots, a_n \in \mathbb{Z}^m \) of the monomials \( x^{a_1}, \ldots, x^{a_n} \in \mathbb{C}[x_1, \ldots, x_m] \) are given fixed. These exponents form the so-called support of the sparse polynomials. The convex hull \( \text{conv}(a_1, \ldots, a_n) \) of the exponents is called the Newton polytope. We assume in the following that the Newton polytope has dimension \( m \) which is the number of variables. (If this is not the case, the Hermite normal form may be used to compute a basis of the lattice and reduce to this situation.) A facet of the Newton polytope is a face of dimension \( m - 1 \). A facet \( F \) is characterized by a linear functional \( \omega : \mathbb{R}^m \to \mathbb{R}, x \mapsto \omega^t x \) (where \( \omega \in \mathbb{R}^m \) is a given vector) such that the linear functional \( \omega \) attains its minimum at the facet. This inner normal is unique up to scaling. By an initial facet system we mean

\[ \text{in}_{\omega}(f_i) = \sum_{a_j \in F_\omega} c_{ij} x^{a_j} = 0, \quad i = 1, \ldots, r, \]

which is derived from the original polynomials \( f_i, i = 1, \ldots, r \), by neglecting the monomials whose exponents are not on the facet \( F_\omega \) of the Newton polytope. Similarly, an initial face system is defined.

Analogue definitions hold if the supports of the polynomials \( f_i \) are different. Assume that there are supports \( A_i, i = 1, \ldots, r \), and thus \( r \) Newton polytopes. Assume there are \( k_i \) polynomials with the same support:

\[ f_{ij}(x) = \sum_{a \in A_i} c_{ja} x^{a} , \quad i = 1, \ldots, r, \quad j = 1, \ldots, k_i. \]

A face of the tuple of polytopes \( \text{conv}(A_i), i = 1, \ldots, r \), is a set of subsets \( F = (F_1, \ldots, F_r) \) with \( F_i \subseteq \text{conv}(A_i), i = 1, \ldots, r \), such that a linear functional \( \omega \) attains for each \( i = 1, \ldots, r \) its minimum over \( \text{conv}(A_i) \) at \( F_i \). If the dimension of the face differs from the
dimension of the tuple of polytopes by one, then the face is called **facet**. Without loss of
generality we assume that the dimension of the Minkowski sum
\[
\sum_{i=1}^{r} \text{conv}(A_i) = \left\{ \sum_{i=1}^{r} b_i \mid b_i \in \text{conv}(A_i) \right\}
\]
is \(m\). By an **initial facet system** we mean
\[
in_\omega(f_{ij}) = \sum_{a \in F_i} c_{ja} x^a = 0, \quad j = 1, \ldots, k_i, \ i = 1, \ldots, r.
\]

Analogously, **initial face systems** are defined.

The **mixed volume** \(\text{MV}(\text{conv}(A_1), \ldots, \text{conv}(A_r), k_1, \ldots, k_r)\) is defined as a coefficient
of a certain polynomial [7, p. 322]. By Bernstein’s theorem [7, p. 331] it is generically
the number of complex solutions in \((\mathbb{C}\{0\})^m\) of a system \(f_{ij}(x) = 0, \ i = 1, \ldots, r, \ j = 1, \ldots, k_i\) with \(k_1 + \cdots + k_r = m\).

In the following theorem we make the restriction generically more precise.

**Theorem 3.1** ([2], Theorem 6.1 in [25]). Given a system of sparse Laurent polynomials \(f_1, \ldots, f_m\) in \(m\) variables with support \(A_1, \ldots, A_r\) where the supports arise with multiplicities \(k_1, \ldots, k_r\). The number of toric solutions \(x \in (\mathbb{C}\{0\})^m\) (counted with multiplicity) equals the mixed volume if and only if the initial facet systems have no non-trivial solutions
in \(\mathbb{C}^m\) or at infinity.

**Remark 3.2.** (a) In [25] the existence of non-trivial solutions is formulated more precisely
in terms of a vanishing sparse resultant. (b) In the original work [2] Bernstein formulated
this criterion for faces instead of facets and demanded the non-existence of non-trivial
affine solutions. (c) Clarke [5] calls the Newton polytope exponent polytope and derives
similar results. These results are also recalled in [6, Chapter VI] but are applied in [6] in a
different way than we do in this article.

**Sketch of Proof.** First we sketch the constructive proof for the case of one support \(A\)
forming the columns of a matrix \(A\). For simplicity we assume that the dimension of the
Newton polytope (and thus also the lattice) is \(m\). The solutions \(x \in (\mathbb{C}\{0\})^m\) may be found
from a line in the intersection of the kernel of the coefficient matrix with the homogeneous
toric variety \(V(I_{\hat{A}})\). Here \(\hat{A}\) is the matrix whose columns are \((1, a_i)\), with \(a_i\) the exponents
of monomials \(x^{a_i}\) and
\[
I_{\hat{A}} = \{ f \in \mathbb{C}[z_1, \ldots, z_n] \mid f(x_0 x^{a_1}, \ldots, x_0 x^{a_n}) = 0, \ \forall x \in (\mathbb{C}\{0\})^m, x_0 \in \mathbb{C} \}.
\]
the homogeneous toric ideal. Rescalings \(\tau \in (\mathbb{C}\{0\})^m, (x_0, x_1, \ldots, x_m) \mapsto (x_0, \tau x_1, \ldots, \tau x_m)\) defines a torus action which induces by the given monomials a torus action on \(\mathbb{C}^n\).
\(V(I_{\hat{A}}) \subseteq \mathbb{P}^{n-1}\) is the Zariski closure of the maximal orbit \(O_1\) of this induced torus action.
(The quotient ring \(\mathbb{C}[z]/I_{\hat{A}}\) is not assumed to be normal as usually in algebraic geometry.
This property is not used in this article.)
If $z$ is generating an intersecting line such that all components $z_i$ are unequal zero then at least one solution $x \in (\mathbb{C}\setminus \{0\})^m$ of (7) is found by solving $x_0x^\lambda = z$ by Hermite normal form or Smith normal form. If $z$ is real and positive then one associated $x$ is positive.

The cases with some $z_i = 0$ are related to the facets of the Newton polytope as follows. Assume $\text{conv}(\mathcal{A})$ has $N$ facets with inner normals $\omega_1, \ldots, \omega_N$. Each inner normal $\omega_i \in \mathbb{Z}^m$ is normalized such that the components $\omega_1, \ldots, \omega_N$ are relatively prime. Denote by $V$ the matrix with rows $\omega_i$. In [7, p. 309] the facet variables $t_1, \ldots, t_N$ are introduced by

$$
x_1 = t_1^{\omega_1}, \ldots, t_N^{\omega_N}, \\
\vdots \\
x_m = t_1^{\omega_m}, \ldots, t_N^{\omega_N}.
$$

(8)

After substitution into the monomials, we obtain new monomials $t^{V_{a_1}}, \ldots, t^{V_{a_N}}$ in the facet variables, whose exponents form the columns of $VA$. Then $Vt_{\hat{A}} = V_{\hat{A}}$. Since a shift of the Newton polytope does not change the homogeneous toric variety one may multiply all monomials by $t^b$ where $-b_j$ is the minimal value of the functional $\mathbb{R}^m \to \mathbb{R}$, $w \mapsto v_j^Tw$ on $\text{conv}(\mathcal{A})$. Then $V_{a_i} + b \geq 0$ and $(V_{a_i} + b)_j = 0$ iff $a_j$ is on the $j$th facet. That means that $(\mathbb{C}\setminus \{0\})^m \to \mathbb{P}^{m-1}, (x_1, \ldots, x_m) \mapsto [x^{a_1} : \ldots : x^{a_N}]$ and $(\mathbb{C}\setminus \{0\})^N \to \mathbb{P}^{n-1}, (t_1, \ldots, t_N) \mapsto [t^{V_{a_1}+b} : \ldots : t^{V_{a_N}+b}]$ are two different parameterizations of the maximal orbit $O_1 \subset V(I_{\hat{A}})$.

The torus group $(\mathbb{C}\setminus \{0\})^N$ is operating non-faithful on $\mathbb{P}^{n-1}$ since the maximal orbit has dimension $m$. Representatives of $(\mathbb{C}\setminus \{0\})^N/(\mathbb{C}\setminus \{0\})^m$ are chosen by setting some $t_i = 1$ in the following way. For a vertex $a_j$ of the Newton polytope we distinguish neighboring facets and non-neighboring facets. All facet variables of non-neighboring facets are chosen to be one. If the inner normals of the neighboring facets are linearly dependent this dependence defines algebraic relations in the facet variables. By this choice $t^{V_{a_j}+b} = 1$. Substitution of $z_j = 1$ into $I_{\hat{A}}$ gives an affine toric ideal.

In [8] it is explained that not too many $t_i$ may vanish at the same time since $[0 : \ldots : 0]$ is not an element of $\mathbb{P}^{n-1}$. The monomial ideal $B = (\langle \prod_{\sigma \in F_1} t_1^{|\sigma|} \mid \sigma \text{ is a face of the Newton polytope} \rangle)$ is generated by monomials where $\sigma(1)$ is the set of facets which have $\sigma$ as a face. Then

$$
\mathbb{C}^N \setminus V(B) \to \mathbb{P}^{n-1}, \quad (t_1, \ldots, t_N) \mapsto [t^{V_{a_1}+b} : \ldots : t^{V_{a_N}+b}]
$$

is a parameterization of $V(I_{\hat{A}})$.

For $t_j = 0$ we have $t^{V_{a_j}+b} = 0$ for all $i_j$ not on the $j$th facet. This reduces the original system $f(x) = 0$ to an initial facet system. This gives a homogeneous toric subvariety corresponding to $a_{v_1}, \ldots, a_{v_s}$, the points on the $j$th facet. Assume there exists $z \in \mathbb{C}^m$ in the kernel of the coefficient matrix with $z_{\mu} = 0$ for all $\mu \notin \{v_1, \ldots, v_s\}$ and $[z] \in V(I_{\hat{A}})$. Then Hermite normal form gives solutions $t \in \mathbb{C}^N$ of

$$
l_0^{V_{a_1}+b} = z_1, \ldots, \quad l_0^{V_{a_N}+b} = z_N.
$$
For backsubstitution with (8) we eventually need projective coordinates \([x_0 : x_1 : \cdots : x_m] \in \mathbb{P}^m\). For an index \(j\) of a facet with \(t_j = 0\) and \(d_j = \min_{\mu \in \{1, \ldots, m\}} \omega_{j\mu} < 0\) rescaling in projective space \(\mathbb{P}^m\) gives

\[
x_0 = t_j^{-d_j},
\]

\[
x_1 = t_j^{\omega_{j1}} \cdot \cdots \cdot t_j^{\omega_{jm}} t_j^{-d_j},
\]

\[
\vdots
\]

\[
x_m = t_j^{\omega_{j1}} \cdot \cdots \cdot t_j^{\omega_{jm}} t_j^{-d_j}.
\]

Substitution of \(t_j = 0\) gives a (generalized) solution with some components being zero or at infinity \((x_0 = 0)\). If the solution \(t\) is real then \([x] \in \mathbb{P}^m\) is real. A real non-negative solution \(t\) with some zero-components corresponds to a real non-negative solution \([x] \in \mathbb{P}^m\) with zero components or at real infinity with non-negative real components.

This corresponds to a solution of the initial facet system \(\mathbf{i}_{\omega_j}(f_i) = 0, i = 1, \ldots, r\).

Since the initial facet system is weighted homogeneous solutions may also be interpreted in the weighted projective space \(\mathbb{P}(\omega_{j1}, \ldots, \omega_{jm})\) where points are identified under the one-dimensional torus action

\[x \mapsto (t_j^{\omega_{j1}} x_1, \ldots, t_j^{\omega_{jm}} x_m).\]

Let us investigate closer the case, where \(f(x) = 0\) has a curve of non-negative real solutions. By homogeneity, the initial facet system has a path of solutions \(p(t_j) = (t_j^{\omega_{j1}} a_1, \ldots, t_j^{\omega_{jm}} a_m), t_j \in (0, \infty), a \in (\mathbb{R}_{\geq 0})^m \setminus \{0\}\) a fixed solution. If the solutions of the original system form a path as well then a local parameterization \(x(t_j), t_j \in (0, \varepsilon),\) satisfies

\[
\lim_{t_j \to 0} \left( \frac{x_1(t_j)}{p_1(t_j)}, \ldots, \frac{x_m(t_j)}{p_m(t_j)} \right) = (1, \ldots, 1).
\]

In the original work [2] the function \(x(t_j)\) is a Puiseux series. Its exponents of the initial terms are given by the inner normal \(\omega\).

We briefly discuss the case that several facet variables vanish, i.e., \(t_{j_1} = \cdots = t_{j_s} = 0\). Then the initial facet system is multihomogeneous with respect to \(\omega_{j_1}, \ldots, \omega_{j_s}\), and the solutions are orbits of the \(s\)-dimensional torus action, i.e., are elements of \((\mathbb{C} \setminus \{0\})^m /(\mathbb{C} \setminus \{0\})^s\). But the limit \(\lim_{t_{j_1} \to 0, \ldots, t_{j_s} \to 0} [1 : x(t)]\) does not exist in \(\mathbb{P}^m\) in general. The theory in [8] explains that this happens if the inner normal fan is not simplicial. Then we use the following trick. The problem is embedded into a larger problem. Additionally, each equation is multiplied with each \(x_i\). Of course this enlarged polynomial system has the same solutions than the original system. The Newton polytope of the new system is the Minkowski sum of the old Newton polytope and the \(m\)-simplex. The projective toric variety associated to the Minkowski sum contains both \(V(I_J)\) and \(\mathbb{P}^m\) as embeddings. Each face of the old Newton polytope gives rise to a face of the new Newton polytope. The same holds true for the \(m\)-simplex. Thus we have
\[ x_1 = t_1^{011} \cdots t_N^{0N1} \tilde{x}_1 / \tilde{x}_0, \]
\[ \vdots \]
\[ x_m = t_1^{01m} \cdots t_N^{0Nm} \tilde{x}_m / \tilde{x}_0, \]

where \( \tilde{x}_0, \tilde{x}_1, \ldots, \tilde{x}_m \) are the facet variables of the \( m \)-simplex. Consider again the situation that an initial face system of the old Newton polytope has a non-trivial solution. This face gives rise to a face of the new Newton polytope, but with different neighboring facets. Some neighboring facets arise from the \( m \)-simplex, giving conditions \( \tilde{x}_i = 0 \) for some \( i \in \{0, 1, \ldots, m\} \). If the limits are uniquely defined (equivalently the inner normal cones are simplicial) then Puiseux series exist.

For several supports \( A_1, \ldots, A_r \), this technique has to be generalized. Finding solutions \( x \in \mathbb{C}^m \) of \( f_i(x) = 0, i = 1, \ldots, r \), is equivalent to finding solutions \( x \in \mathbb{C}^{m+r-1} \) of \( f_1(x) + x^{-2}f_2(x) + \cdots + x^{-r}f_r(x) = 0 \) where \( x^{-2}, \ldots, x^{-r} \) are arbitrary. The multihomogeneous toric ideal

\[ I_{\tilde{\lambda}} = \{ f \in \mathbb{C}[z] \mid f(x_0 x^{a_1}, \ldots, x_0 x^{-i} x^{a_i}, \ldots, x_0 x^{-r} x^{a_r}) = 0, \forall x, x_0, x^{-i} \}, \]

and its variety are used. The lifting is

\[ \tilde{\lambda} = \begin{pmatrix}
1 & \cdots & 1 & \cdots & 1 & \cdots & 1 \\
0 & \cdots & 0 & 1 & \cdots & 1 & \cdots & 0 \\
\vdots & & & & & & & \vdots \\
0 & \cdots & \cdots & \cdots & 1 & \cdots & 1 \\
a_1 & \cdots & \cdots & \cdots & a_n
\end{pmatrix}. \]

The facet variables are now defined by the facets of the tuple of Newton polytopes.

**Remark 3.3.** (a) The proof nicely reflects the structure of the toric variety as a Zariski closure of a maximal orbit. The boundary consists of toric subvarieties which are Zariski closures of orbits of lower dimension. (b) The proof also shows that the protective toric variety is glued together from affine toric varieties. For each vertex of the Newton polytope there is an affine toric variety. All these are identified on the maximal orbit. (c) The one-dimensional torus action \( x \mapsto (t_1^{a_{j1}} x_1, \ldots, t_m^{a_{jm}} x_m) \) has been used numerically in [27]. (d) The technique for several Newton polytopes is usually referred to as Cayley trick [22].

### 3.2. Applications with one Newton polytope

For the system of equations (5), we know about real non-negative solutions of subgraph subsystems by the knowledge of the minimal generators of the convex polyhedral cone \( \ker(Y_k I_k) \cap (\mathbb{R}_{\geq 0})^r \). If such a circuit subsystem is an initial face system, then we found a real solution with some components zero or at infinity (in the real projective space).

Recall that the columns of \( Y_k \) are called \( \eta_1, \ldots, \eta_n \). The Newton polytope of \( Y_k I_k \Psi(x) = 0 \) is the convex hull of \( \{ \eta_i \mid \exists C_i \rightarrow C_j \} \). In other words the Newton polytope is the convex hull of the columns of \( Y_k \).
Definition 3.4. Take a vector \( v \in \mathbb{C}^l \) with some components being zero and recall the definition \( S_v = \{ j \in \{1, \ldots, n\} | \exists \mu \in \{1, \ldots, l\} \text{ with } (I_K e_j)_\mu \neq 0 \text{ and } v_\mu \neq 0 \} \) of initial vertices associated to the support of \( v \). For \( v = I_K \Psi(x) \) these vertices correspond to monomials. We call \( x^{\eta_j}, j \in S_v \), the support monomials of \( v \).

For minimal generators \( E_i \) of the convex polyhedral cone \( \text{ker}(Y_s I_a) \cap (\mathbb{R}_{\geq 0})^l \), we have obviously \( \{ \eta_j | j \in S_{E_i}\} \subset \{ \eta_i | \exists C_i \rightarrow C_j \} \), i.e., all support monomials appear in \( Y_s I_a I_K \Psi(x) = 0 \).

Theorem 3.5. Consider system (5) of sparse polynomials \( Y_s I_a I_K \Psi(x) = 0 \) given by a weighted directed graph and a weighted bipartite graph as defined in Section 2. Let \( \text{conv}(\{ \eta_i | \exists C_i \rightarrow C_j \}) = \text{conv}(\eta_1, \ldots, \eta_r) \) be the Newton polytope. Let \( E_i \) be a minimal generator of the convex polyhedral cone \( \text{ker}(Y_s I_a) \cap (\mathbb{R}_{\geq 0})^l \) and assume the following conditions.

(i) \( E_i \) is a positive circuit in the directed graph.
(ii) There is a face \( F \) of the Newton polytope such that \( F \cap \{ \eta_1, \ldots, \eta_r \} = \{ \eta_j | j \in S_{E_i}\} \). That means the support of \( E_i \) forms a face.
(iii) The points in the support \( \{ \eta_j | j \in S_{E_i}\} \) are affine linearly independent.
(iv) Each vertex of the directed graph associated to a support monomial of \( E_i \) is the initial vertex of an arrow exactly once. That means the support of \( E_i \) forms a terminal strong connected component of the directed graph.

Then the system \( Y_s I_a I_K \Psi(x) = 0 \) has a non-negative real solution with some components zero or infinity.

Proof. The proof is a variation of the proof of Theorem 3.1.

The nullspace \( \text{ker}(Y_s I_a) \) intersects the deformed toric variety on coordinate hyperplanes. By (iii) the projective toric variety for this face is just the projective space itself. By (iv) the linear equations in the deformed toric ideal vanish for the face. By (i) there is a line in the intersection of the homogeneous deformed toric variety with the kernel of the coefficient matrix. Since the generator \( E_i \) of the line is non-negative the solutions of the facet variables are non-negative and thus the \( x_i \) are non-negative.

Next we give criteria for condition (ii), i.e., for the support \( S_{E_i} \) to be a face. In general, this is a difficult combinatorial task. But here we exploit the additional structure of sparsity of monomials. Analogous to the support of a vector, we define the notion of the support of a monomial.

Definition 3.6. For a Laurent monomial \( x^a \) in the variables \( x_1, \ldots, x_m \) the support is \( T(x^a) = \{ j \in \{1, \ldots, m\} | a_j \neq 0 \} \) and the \( x_j \) with \( j \in T(x^a) \) are the support variables.

Lemma 3.7. Given \( \eta_i \in (\mathbb{Z}_{\geq 0})^m, i = 1, \ldots, r, \) and \( S \subset \{1, \ldots, r\} \) with a set of points \( \eta_i, i \in S \). Suppose the supports \( T(x^{\eta_i}) \) for \( i \in S \) and for \( i \in \{1, \ldots, r\}\setminus S \) satisfy the following statement.
Proof. We construct explicitly a linear functional $\omega$ which attains its minimum at the points associated to $S$ and is larger outside. For all support variables $x_k$ of monomials $x^{\eta_j}$, $j \in S$, we set $\omega_k = 0$. For all other variables we set $\omega_k = 1$. Then $\omega(\eta_j) = 0$ for all $j \in S$. For $\eta_i$, $i \notin S$, there is a variable $x_k$ with $\omega_k > 0$ and $(\eta_i)_k > 0$ by condition (C). Thus the support of $S$ forms a face. \hfill \square

Remark 3.8. (a) An equivalent formulation for (C) is the condition that all points associated to $S$ lie in one coordinate hyperplane and the others above. (b) For chemical reaction systems the set $S$ is a collection of complexes (vertices of the bipartite graph). Condition (C) may also be formulated as a property of the reduced bipartite graph associated to $Y_r$. (C) means that the set of vertices $S_i$ decomposes into two subset. One set of vertices being adjacent to a vertex $C_j$ with $j \in S$ and one subset of vertices which are not adjacent.

Lemma 3.9. Given $\eta_i \in (\mathbb{Z}_{\geq 0})^m$, $i = 1, \ldots, r$, and $S \subset \{1, \ldots, r\}$ with a set of points $\eta_i$, $i \notin S$. Suppose the supports $T(x^{\eta_i})$ for $j \in S$ and for $i \in \{1, \ldots, r\}\setminus S$ satisfy the statements (D) and either (C+) or (C-).

(D) The supports of the monomials in $S$ are all different or all monomials of $S$ have the same weighted degree. That means for all $i$, $j \in S$ either
\begin{itemize}
  \item $T(x^{\eta_i}) \cap T(x^{\eta_j}) = \emptyset$ and $T(x^{\eta_i}) \neq \emptyset$ or $T(x^{\eta_j}) \neq \emptyset$ or
  \item for all $k \in T(x^{\eta_i}) \cap T(x^{\eta_j})$ the degrees satisfy $\deg_k(x^{\eta_i}) = \deg_k(x^{\eta_j})$ and $\deg_W(x^{\eta_i}) = \deg_W(x^{\eta_j})$.
\end{itemize}
Here, the weighted degree is given by the degree of $x_k$ in a monomial, $\deg_k(x^{\eta_i}) = \eta_{ki}$, and $W$ defines some other weighted degree.

(C+) All monomials $x^{\eta_i}$ outside (i.e., $i \notin S$) have a support which is either not contained in the union of supports of $S$ or the monomial has larger weighted degree. That means for all $i \in \{1, \ldots, r\}\setminus S$ either $T(x^{\eta_i}) \not\subseteq \bigcup_{j \in S} T(x^{\eta_j})$ or $\deg_W(x^{\eta_i}) > \deg_W(x^{\eta_j})$, $\forall j \in S$.

(C-) All monomials $x^{\eta_i}$ outside (i.e., $i \notin S$) have a support which is either not contained in the union of supports of $S$ or the monomial has smaller weighted degree. That means for all $i \in \{1, \ldots, r\}\setminus S$ either $T(x^{\eta_i}) \not\subseteq \bigcup_{j \in S} T(x^{\eta_j})$ or $\deg_W(x^{\eta_i}) < \deg_W(x^{\eta_j})$, $\forall j \in S$.

Then the points $\eta_j$, $j \in S$, generate a face of the Newton polytope. More precisely, there is a face $F$ of the Newton polytope such that $F \cap \{\eta_1, \ldots, \eta_r\} = \{\eta_i \mid i \in S\}$.

Proof. We construct explicitly a linear functional $\omega$ which attains its minimum at the points associated to $S$ and which is larger outside. By (D) we can define a weighted degree
by $\deg_W(x_k) = \deg_k(x^\eta_j)$, $k \in T(x^\eta_j)$, for all variables of $\bigcup_{j \in S} T(x^\eta_j)$. Let $d$ be the product of the degrees of the monomials $x^\eta_j$ for the set $S$. In formulas $d := \prod_{j \in S} \deg_W(x^\eta_j)$.

For each variable $x_k$ in the support $T(x^\eta_j)$ of $j \in S$ we define $\omega_k = \sigma d / \deg_W(x^\eta_j)$, where $\sigma = 1$ in case $(C^+)$ is valid and $\sigma = -1$ for the case $(C_-)$. This is well defined because of condition (D). Then $\omega_j = \sigma d$ for $j \in S$.

$(C^+)$ All other variables $x_j$ get $\omega_j = d + 1$. By $(C^+)$ first case for a point $\eta_j$ outside $S$ there is a variable $x_k$ with $k \notin \bigcup_{j \in S} T(x^\eta_j)$. For this $\omega_k = d + 1$ and $(\eta_k)_k \neq 0$. Thus $\omega_j \eta_j \geq d + 1$. For the second case $\deg_W(x^\eta_j) > \deg_W(x^\eta_i)$ guarantees $\omega_j \eta_j > d$.

$(C_-)$ For a variable $x_\nu$ which is not in the union of supports of $S$, but in a support of a monomial outside $S$ which contains a support of a monomial in $S$ we define $\omega_k = 1$. All other variables get weight zero.

Remark 3.10. (a) The condition (D) can be reformulated by saying that all points associated to $S$ lie in one coordinate hyperplane. They generate a polytope of dimension less than the dimension of the coordinate hyperplane. Conditions $(C^+)$ and $(C_-)$ mean that all other points either lie above the coordinate hyperplane or lie outside the polytope generated by $S$. All exceptional points inside the coordinate hyperplane lie all above or below the polytope. (b) For chemical reaction systems the set $S$ is a collection of complexes (vertices of the bipartite graph). Then conditions (D), $(C^+)$ and $(C_-)$ can be formulated as properties of the reduced bipartite graph associated to $Y_r$. $(C^+)$ and $(C_-)$ mean that the set of vertices $S_j$ decomposes into two subsets, one subset of vertices being adjacent to an $C_j$, $j \in S$, and the set of the remaining vertices $S_k$. For a $C_j$, $j \notin S$, there is an adjacent remaining $S_k$ or the weighted sum of incident edges is different. Condition (D) means that for two vertices $C_i$ and $C_j$ either there is no vertex $S_k$ which is adjacent to both $C_i$ and $C_j$, or if $S_k$ is adjacent to both then the two edges have same weight $\eta_{ki} = \eta_{kj}$ and the sum of weights of incident edges is equal for both $C_i$ and $C_j$.

The results are summarized in the following way. Under weak additional conditions circuit subsystems are initial face systems.

Fig. 3. A small model for reactions on the surface of a metal.
Example 3.11. The first example in [10] is illustrated in Fig. 3. The exponents are the columns of the matrix

\[
Y_s = Y_k = \begin{pmatrix}
1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 \\
0 & 2 & 0 & 1 & 0 & 3
\end{pmatrix}
\]

giving the equations

\[
0 = -k_{2,1} x_1 + k_{1,2} x_3^2 - k_{6,5} x_1 x_2, \\
0 = -k_{4,3} x_2 + k_{3,4} x_3 - k_{6,5} x_1 x_2, \\
0 = 2k_{2,1} x_1 - 2k_{1,2} x_3^2 + k_{4,3} x_2 - k_{3,4} x_3 + 3k_{6,5} x_1 x_2.
\]

The conservation relation is \(2 x_1 + x_2 + x_3 - c_1 = 0\) with \(v_1 = (2, 1, 1)\). The toric ideal is \(I_{\mathcal{F}} = \langle w_1 w_2 w_3 - w_4^2 w_5 \rangle\) while the deformed toric ideal is \(I_{\mathcal{F}}^{\text{def}} = \langle k_{2,1}^2, k_{6,5} z_1 z_2 z_3 - k_{2,1} k_{3,4} z_2^2 z_3 \rangle\). There are two positive circuits, namely \(E_1 = (1, 1, 0, 0, 0)\) and \(E_2 = (0, 0, 1, 1, 0)\). Each of them gives rise to a face of the Newton polytope \(\text{conv}(\eta_1, \ldots, \eta_5)\) (Fig. 4). Using facet variables

\[
x_1 = t_1 t_2 t_5^{-2}, \quad x_2 = t_1 t_3 t_6^{-2}, \quad x_3 = t_1 t_4 t_5^{-1} t_6^{-1},
\]

we compute the irrelevant ideal \(B = \{t_1, t_2 t_6, t_3 t_5, t_5 t_6, t_1 t_2 t_3\}\) and \(V(B) = \{t_1 = t_2 = t_5 = 0\text{ or } t_1 = t_3 = t_6 = 0\text{ or } t_1 = t_5 = t_6 = 0\}\). We investigate two limits. For \(E_1\) we choose \(t_1 = t_2 = t_6 = 1\) and study the limit \(t_3, t_5 \to 0\) giving the initial face system \(k_{2,1} x_1 - k_{1,2} x_3^2 = 0\)
or equivalently $k_{2.1}t_5^{-2} - k_{1.2}t_5^{-2} = 0$. The solutions form a two-dimensional set since the equations are homogeneous with respect to two weighted gradings. The limit is

$$
\lim_{t_3, t_5 \to 0} \left[ \begin{array}{c} 1 : \frac{1}{t_5} : t_5 : \sqrt[\frac{2}{t_1, t_5}} \end{array} \right] = \lim_{t_3, t_5 \to 0} \left[ \begin{array}{c} t_2^2 : 1 : t_3 t_5^2 : \sqrt[\frac{2}{t_1, t_5}} \end{array} \right] = [0 : 1 : 0 : 0].
$$

For $E_2$ we choose $t_3 = t_4 = t_5 = 1$. The limit $t_1, t_2 \to 0$ gives the initial face system $k_{4,3}x_2 - k_{3,4}x_3 = 0$ or equivalently $k_{4,3}t_6^{-2} - k_{3,4}t_6^{-1} = 0$ yielding $t_6 = k_{4,3}/k_{3,4}$. The limit is the origin.

The chemical interpretation is the following. In the first limit the amount of the first species is infinite such that no space on the surface is left and only the first forward–backward reaction may be performed. In the second limit there is no available space. For very small amount of space first the second reaction pair is performed since $x^{\eta_2} = x_2$ has lower degree than $x^{\eta_1} = x_1$.

**Example 2.1 (continued).** In this example we have

$$
Y_k = (\eta_1, \ldots, \eta_{11}) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 \end{pmatrix}.
$$

The Newton polytope is generated by $\eta_1, \eta_3, \eta_4, \eta_6, \eta_7, \eta_8, \eta_9, \eta_{10}$ since $C_2, C_5, C_{11}$ are pure product complexes. The deformed toric ideal $I_k^{\text{def}}$ is

$$
\langle k_{5,4}z_4 - k_{9,4}z_5, k_{7,11,8,7,2,2,6} - k_{9,3}k_{10,6}z_3^2, k_{9,3}k_{10,7}k_{7,10}z_7^2 z_3 - k_{2,4}k_{3,9}z_2^2 z_7 z_8 \rangle.
$$
The convex polyhedral cone is generated by 5 vectors including 3 stoichiometric generators:

\[ E_1 = [0, 1, 0, 0, 0, 0, 0, 0], \quad E_2 = [0, 0, 0, 0, 0, 1, 1, 0]. \]

Their supports are \( S_{E_1} = \{3, 9\} \) and \( S_{E_2} = \{7, 10\} \), because \( v_2 = k_{9.3}x^{10} \), \( v_3 = k_{3.9}x^{10} \), \( v_7 = k_{10.7}x^{10} \), \( v_8 = k_{7.10}x^{10} \). By Lemma 3.9 the support of \( E_1 \) generates a face of the Newton polytope as well as the support of \( E_2 \) does. \( \omega_1 = (2, 1, 3, 2, 2) \) attains its minimum on the face \( \text{conv}(\eta_3, \eta_9) \) while \( \omega_2 = (-2, 1, 1, 0, -2) \) attains its minimum on the face \( \text{conv}(\eta_7, \eta_10) \).

The 5-dimensional Newton polytope has 8 facets, \( F_i, i = 1, \ldots, 8 \). According to (8), this gives the coordinate transformation with facet variables \( t_i, i = 1, \ldots, 8 \),

\[
\begin{align*}
x_1 &= \frac{t_6 t_7}{t_5^2}, & x_2 &= \frac{t_6 t_8}{t_2 t_5}, & x_3 &= \frac{t_4 t_6^2}{t_2^2 t_5^2}, & x_4 &= \frac{t_3 t_6}{t_2 t_5}, & x_5 &= \frac{t_1 t_6^2}{t_2 t_5^2}.
\end{align*}
\]

In order to determine the exceptional set \( V(B) \) we determined the 86 faces and computed a Gröbner basis yielding

\[ B = \{ t_3, t_4, t_1 t_6, t_2 t_7, t_5 t_8, t_1 t_2 t_5, t_6 t_7 t_8 \}. \]

The monomials in facet variables are

\[ \Psi(t) = \left( t_6 t_7^2 t_8^2, \frac{t_6 t_8}{t_2 t_5}, t_2^2, t_8^2, t_4, \frac{t_2 t_4}{t_6}, t_3^2, t_2^2, t_5 t_8 t_3, t_2 t_5 t_1, \frac{t_2^2}{t_6^2}, \frac{t_4^2}{t_5} \right). \]

The vector \( v \) in facet variables is

\[ v(t) = \left( k_2.1 t_6 t_7 t_8^2, k_9.3 t_2^2 t_8^2, k_3.9 t_2^2 t_5^2 t_1, k_9.4 t_4, k_5.4 t_4, k_{10.6} t_5^2, k_{10.7} t_2^2 t_7, k_{11.8} t_8 t_3 \right). \]

For \( E_1 \) we computed that the vertex \( \eta_3 \) lies on the facets \( F_1, F_2, F_3, F_4, F_5, F_6, F_7 \) while \( \eta_9 \) lies on the facets \( F_3, F_4, F_6, F_7, F_8 \). The edge \( \{\eta_3, \eta_9\} \) is the intersection of the facets \( F_3, F_4, F_6, F_7, F_8 \). We choose a chart of the protective toric variety by restricting to \( t_1 = t_2 = t_5 = 1 \). Then the initial face system corresponding to \( E_1 \) is \( k_{3.9}x_2^2 - k_{9.3}x_5 = 0 \) or equivalently \( k_{9.3}t_2^2 - k_{3.9} = 0 \). We substitute \( t_3 = t_4 = t_6 = t_7 = 0 \) into (9) which yields the limit \( x = 0 \). The associated constant in the conservation relation is \( c_1 = 0 \). This agrees with the understanding of chemists. If no free space on the surface is available then the concentrations of all substances on the metal are zero. Since no reactions happen the concentration of \( \text{H}_2\text{O} \) is zero too.

For \( E_2 \) the computation yields that \( \eta_7 \) is on the facets \( F_1, F_3, F_4, F_5, F_6, F_8 \) while \( \eta_{10} \) is on the facets \( F_2, F_3, F_4, F_5, F_7, F_8 \). The edge \( \{\eta_7, \eta_{10}\} \) is the intersection of the facets \( F_3, F_4, F_5, F_8 \). Unfortunately, both inner normal cones of \( \eta_7 \) and \( \eta_{10} \) are not simplicial. Choosing the vertex \( \eta_{10} \) enables us to restrict to \( t_1 = t_6 = 1 \). The initial face system
Proposition 3.12. Assume the system (5) of sparse polynomials \( Y_s I_a I_K \Psi(x) = 0 \) is given by a weighted directed graph and a weighted bipartite graph as defined in Section 2. Let \( E_i \) and \( E_j \) be two different minimal generators of the convex polyhedral cone \( \ker(Y_s I_a) \cap (\mathbb{R}_{\geq 0})^j \) and assume the following conditions.

(i) \( E_i \) and \( E_j \) are positive circuits in the directed graph.
(ii) The exponents of the support-monomials of \( E_i \) and \( E_j \) generate a face of the Newton polytope.
(iii) The points in the supports \( \{ \eta_j \mid j \in S_{E_i} \cup S_{E_j} \} \) are affine linear independent.
(iv) The supports of \( E_i \) and \( E_j \) form a terminal strong connected component of the directed graph.

Then the system \( Y_s I_a I_K \Psi(x) = 0 \) has a non-negative real solution with zero-components or infinity.

More generalizations of Theorem 3.1 including several positive circuits are easily formulated.
Example 3.13. The following chemical reaction is taken from [30] where it is left for further research. It models non-competitive inhibition.

\[
\begin{align*}
S + E & \longleftrightarrow C_1 \longleftrightarrow P + E \\
C_1 + I & \longleftrightarrow C_2 \longleftrightarrow C_3 + S \\
E + I & \longleftrightarrow C_3
\end{align*}
\]

There are 7 species. Thus the Newton polytope is a subset of \(R^7\). But it has dimension 6 and thus the lattice is degenerate. The vector space of conservation vectors has dimension 3. Since the lattice is degenerate the real variety in the positive orthant is always transversal to the affine spaces given by the conservation relation

\[
x_E + x_{C_1} + x_{C_2} + x_{C_3} - c_1 = 0.
\]

The two other relations are

\[
\begin{align*}
x_I + x_{C_2} + x_{C_3} - c_2 & = 0, \\
x_S + x_{C_1} + x_P + x_{C_2} - c_3 & = 0.
\end{align*}
\]

The first two components of the directed graph correspond to faces of the Newton polytope by Proposition 3.12 while the last component forms a face by Lemma 3.9. Using the facet variables of the Minkowski sum of the Newton polytope and a 7-simplex we obtain three limits for

\[
\begin{bmatrix}
\mathbf{w}_7(t_6) & \mathbf{k}_1 & \mathbf{k}_2 & \mathbf{k}_3 \\
\mathbf{w}_7(t_14) & \mathbf{k}_4 & \mathbf{k}_5 & \mathbf{k}_6 & \mathbf{k}_7
\end{bmatrix}
\]

1 component:

\[
\lim_{t_6 \to 0} \begin{bmatrix}
w_7t_6 & k_{1,1} & w_7 & k_{1,2} & k_{1,3} & w_7 & 0 & 0
\end{bmatrix}.
\]

2 component:

\[
x_0 = 0, \quad x_E = 0, \quad x_P = 0,
\]

3 component:

\[
\lim_{t_{14} \to 0} \begin{bmatrix}
w_7t_{14} & k_{7,1} & 0 & 0 & 0 & w_7 & 0 & 1
\end{bmatrix}.
\]

For the first component the limit corresponds to \(c_2 = 0\) while for the last component the limit corresponds to \(c_3 = 0\).

We summarize the results of this section as follows. Under weak assumptions, subgraph subsystems corresponding to terminal strong connected components are initial face systems. This means the steady states of the full system (5) for extreme values of the conservation constants \(c_i\), are determined by these subgraph subsystems.

### 3.3. Several Newton polytopes

In this subsection we distinguish the different supports \(\mathcal{A}_i, i = 1, \ldots, m\), of the single equations in \(Y_tI_iI_k\Psi(x) = 0\).

By Theorem 3.1 we need to consider initial facet systems of the tuple of Newton polytopes. Observe that polynomials whose coefficients have all the same sign do not have real positive solutions. In order to find real positive solutions of the initial facet system a necessary requirement is that the signs of coefficients differ.

**Definition 3.14.** Given sparse polynomials \(f_{ij} = \sum_{a \in A_i} c_{ij}x^a \in \mathbb{R}[x_1, \ldots, x_m], i = 1, \ldots, r, j = 1, \ldots, k_i, \sum_i k_i = m = \dim(\text{conv}(\mathcal{A}_1) + \cdots + \text{conv}(\mathcal{A}_r)). A facet \(F = \)
The signed Newton polytopes of our chemical reaction system (5) have special properties. Often the dimension satisfies \( \dim(\text{conv}(\mathcal{A}_i)) < m \). Often the support of one equation is the union of the supports of some other polynomials.

Observe that the support of the \( i \)th equation can be read off from the combined graph. The reaction complexes \( C_j \) being adjacent to \( S_i \) in the bipartite graph give monomials with negative coefficient. Each arrow \( C_k \rightarrow C_j \) in the directed graph with an \( C_j \) being adjacent to \( S_i \) give a monomial with positive coefficient. So all monomials \( x^{\eta_j} \) above \( (\eta_{ij} > 0) \) have negative coefficient while all monomials below \( (\eta_{ij} = 0) \) have positive coefficient. For an example see Fig. 4.

The efficient computation of all alternating facets for a chemical reaction system (5) is left for future research.

Observe that each forward–backward reaction gives a pair of monomials with one negative and one positive coefficient. The polynomials contain either both monomials or none of them. Thus they are good candidates for the components \( F_i \) of alternating faces.

**Lemma 3.15.** Consider a terminal strong connected component of the directed graph consisting of forward–backward reactions such that its complexes \( C_j \), \( j \in S \), satisfy conditions (D) and either \((C^+)\) or \((C^-)\) of Lemma 3.9. Then the tuple of Newton polytopes has an alternating face \( F = (F_1, \ldots, F_r) \).

**Proof.** By Lemma 3.9, \( \text{conv}(\eta_j, j \in S) \) is a face of the full Newton polytope. Thus for \( i \) with \( \text{conv}(\eta_j, j \in S \cap \mathcal{A}_i) \neq \emptyset \), it is a face of the Newton polytope \( \text{conv}(\mathcal{A}_i) \) for all \( i \in A = \bigcup_{j \in S} T(x^{\eta_j}) \). This defines a cone of directions \( \omega \) attaining its minimum at the face of these \( \text{conv}(\mathcal{A}_i) \). Since the terminal strong connected component consists of forward–backward reactions for each \( i \in A \) there is a pair \( C_j \leftrightarrow C_k \) with \( j, k \in F_i \) whose coefficients of the associated monomials have different sign. Each \( \omega \) in the cone attains its minimum over the other \( i \notin A \) in at least one point. \( \square \)

**Example 3.11 (continued).** The two faces of the full Newton polytope give rise to two facets of the tuple of the Newton polytopes, see Fig. 6. \( \omega_1 = (-2, 1, -1) \) defines the facet \( (|C_1, C_2|, |C_4, C_5|, |C_1, C_2|) \) while \( \omega_2 = (2, 1, 1) \) defines the facet \( (|C_1, C_2|, |C_3, C_4|, |C_3, C_4|) \). Both are alternating and have positive solutions. This makes the results from one Newton polytope in Fig. 5 more precise. With one Newton polytope we saw that the curve is approaching two hypersurfaces in their limits. Distinguishing several Newton polytopes we obtain that the curve is approximating the curves \( (\frac{1}{2}, t^{-2}, \frac{1}{2}, 1, t^{-1}) \) and \( (\frac{1}{2}, t^2, \frac{1}{2}, 1, t) \) on these hypersurfaces.

Besides terminal strong connected components also other structures of mass action kinetics lead to alternating faces. For example in [17] the authors discuss a chemical reaction with a so-called starter radical. This phenomenon is left for future research.
3.4. New results on positive solutions

The following theorem shows that the technique of alternating faces can be used to prove the existence of positive steady states for all parameter values.

**Theorem 3.16.** Assume a system with one conservation relation with $v_1 > 0$. Assume the solutions of $Y_1 I_a I_K \Psi(x) = 0$ form a curve. Assume that one limit is $x = 0$ and one is non-negative infinity and that there are no other alternating cells with non-negative solutions. Then the system

$$Y_1 I_a I_K \Psi(x) = 0, \quad v_1' x - c_1 = 0$$

has at least one positive solution for all possible choices of $k_{ij} > 0$ and $c_1 > 0$.

**Example 2.** This example is an instance of the theorem. Computations show that there are two alternating facets of the tuple of Newton polytopes induced by $E_1$ and $E_2$ such that the initial facet system has a positive solution. The total number of facets is 29. But, all other facets are either not alternating or do not have a positive solution. Thus the real curve links the origin with positive infinity. There is at least one solution of system (5) and (6) for each positive value of the rate constants $k_{ij}$ and for each positive value of the constant $c_1$ in the conservation relation.

Similar versions of Theorem 3.16 are easily formulated. The same principle is valid for several conservation relations, restrictions for the constants in the conservation relations, and for higher dimension of the real variety of $Y_1 I_a I_K \Psi(x) = 0$.

**Example 3.** For the case of one Newton polytope we saw three facets whose initial face system has affine non-negative solutions. If we distinguish the supports of the single equations we find that the tuple of Newton polytopes has many alternating facets. Among these there are three facets corresponding to the connected components.
whose initial facet system has a non-trivial solution. All other can be neglected. This polynomial system has for each positive value of the constants $c_1, c_2, c_3$ a positive solution.

These results agree with the fact that a system with mass action kinetics has a non-negative solution in each space \( \{ x \in (\mathbb{R}_{\geq 0})^m \mid v_i^T x - c_i = 0, i = 1, \ldots \} \), provided they are bounded, see [28].

4. Multistationarity by Viro’s method

In this section we clarify the importance of stoichiometric generators $E_i$ and its confluent vectors $g_i = I_a E_i \neq 0$ for the presence of several positive solutions (multistationarity). We restrict to the case $Y = Y_s = Y_k \in (\mathbb{Z}_{\geq 0})^{m,n}$. Multistationarity happens in the limit $k_{ij} \to 0$ for some $k_{ij}$. In this limit the polynomial system (5) deforms to stoichiometric subgraph subsystems where Clarke’s cone is generated by just one stoichiometric generator.

We start by discussing rescalings of the rate constants $k_{ij}$.

Lemma 4.1. As in Section 2 we assume two graphs which define the system (5) and (6) with mass action kinetics. If $a \in \mathbb{R}^m_+$ is a solution of the unscaled system (5) and (6) then the scaled point $\tilde{a} = \text{diag}(\tau_1, \ldots, \tau_m) a$ is a solution of the scaled system

\[
0 = Y I_a I_{\tilde{K}} \Psi(\tilde{x}), \quad 0 = \tilde{v}_i^T \tilde{x} - c_i
\]

where $\tau_i \in \mathbb{R}_+$, $i = 1, \ldots, m$, and

\[
I_{\tilde{K}} = I_K \text{diag} \left( \frac{1}{\Psi_1(\tau)}, \ldots, \frac{1}{\Psi_n(\tau)} \right), \quad \tilde{v}_i = \text{diag} \left( \frac{1}{\tau_1}, \ldots, \frac{1}{\tau_m} \right) v_i.
\]

Remark 4.2. $\tilde{v}_i$ is in general not orthogonal to $\text{im}(Y I_a I_{\tilde{K}})$. Thus the equivalent system is not of the form mass action kinetics as defined in Section 2.

We consider different rescalings of the rate constants $k_{ij}$ which are equivalent to rescalings of $x$ and $v_i, c_i$. The first type of rescaling is $k_{ij} \mapsto \tau k_{ij}$ for all arrows. Then Eq. (5) can be divided by $\tau$ and the system of polynomial equations does not change. The second rescaling $k_{ij} \mapsto \tau^{y_i} k_{ij}$ for all arrows is equivalent to $x \mapsto (x_1, \ldots, x_i / \tau, \ldots, x_m)$ and $v_i \mapsto ((v_i)_1, \ldots, (v_i)_i \tau, \ldots, (v_i)_m)$. A combination of these rescalings is $k_{ij} \mapsto \tau^{y_i / k_{ij}}$ for all arrows. It is equivalent to $x \mapsto (x_1 / \tau, \ldots, x_m / \tau)$ and $c_i \mapsto c_i / \tau$.

So we need to distinguish two different processes. One rescaling of $k_{ij}$ which is equivalent to rescaling of $x$. The other one is given by choosing a representative of $\mathbb{C}^{l-1} / \text{im}(\mathbb{C}^R)$ where $R = \dim(\text{span}(y_2 - y_1, \ldots, y_r - y_1))$ is the dimension of the lattice and $r$ the number of reactant complexes.

According to this we suggest a change of coordinates from $k$ to $k_{\text{new}} = (k_0, \hat{k}_1, \ldots, \hat{k}_R, \hat{k}_1, \ldots, \hat{k}_{l-R-1})$ by
\[ k_j = \prod_{i=1}^{l} (b_{ij})^{\tilde{b}_{ij}}, \quad j = 1, \ldots, l, \quad \tilde{k}_j = \prod_{i=1}^{l} \tilde{b}_{ij}, \quad j = 1, \ldots, l, \]  

where \( B = (b_{ij}) \in \mathbb{Z}^{l \times l} \) is invertible with inverse \( B^{-1} = C = (c_{ij}) \in GL(l, \mathbb{Q}) \). The first row of \( B \) consists of one’s. The \( i \)th row of \( B \) is given by the degrees of monomials in the variable \( x_i \). Given a directed graph and bipartite graph as defined in Section 2. Assume that each connected component of the directed graph is strongly connected. There exists a row of \( B \) many degrees of freedom. Then the deformed toric ideal \( I_{\tilde{A}} \) depends on \( \tilde{k}_j \) only. Then a rescaling of \( x_j \) is equivalent to a rescaling of \( \tilde{k}_j, i = 1, \ldots, R \). We refer to \( \tilde{k}_i, i = 1, \ldots, R \), as toric rate constants.

In the following lemma we are dealing with solutions of \( I_{\tilde{A}} \Psi(x) = 0 \) which are obviously solutions of \( Y \tilde{A} I_{\tilde{A}} \Psi(x) = 0 \). By Lemma 5.1 in [21] the system \( I_{\tilde{A}} \Psi(x) = 0 \) can only have positive solutions if each connected component of the directed graph is strongly connected, see also [24,30]. The content of the following lemma is basically Theorem 2.16 and Lemma 3.6 in [30], see also [24]. In order to understand the relevant mathematical structure we give an alternative algebraic proof based on the Cayley trick [22].

We first recall the idea of the Cayley trick for two polynomials in \( \mathbb{C}[x_1, \ldots, x_m] \): \( f_1(x) = c_1 x^{a_1} + \cdots + c_n x^{a_n}, f_2(x) = c_{n+1} x^{a_{n+1}} + \cdots + c_L x^{a_L} \). A vector \( z \) in the nullspace of the coefficient matrix, i.e., \( c_1 z_1 + \cdots + c_n z_n = 0, c_{n+1} z_{n+1} + \cdots + c_L z_L = 0 \) is a representative \( z \) of a class \([z] \in \mathbb{P}^{n-1} \times \mathbb{P}^{L-1}\). It gives a solution \( x \) by solving the overdetermined system

\[
\begin{align*}
  z_1 &= x_0 x^{a_1}, \\
  \frac{z_2}{a_1} &= x^{a_2-a_1}, \quad \ldots, \quad \frac{z_l}{a_1} = x^{a_l-a_1}, \\
  z_{n+1} &= x_1 x^{a_{n+1}}, \\
  \frac{z_{n+2}}{a_{n+1}} &= x^{a_{n+2}-a_{n+1}}, \quad \ldots, \quad \frac{z_L}{a_{n+1}} = x^{a_L-a_{n+1}}.
\end{align*}
\]

This has a solution if \( z \in V(I_{\tilde{A}}) \subset \mathbb{P}^{n-1} \times \mathbb{P}^{L-1} \) where \( \tilde{A} \) means a double lifting of \( A \) corresponding to two slack variables \( x_0, x_{-1} \):

\[
\tilde{A} = \begin{pmatrix}
  1 & \ldots & 1 & 0 & \ldots & 0 \\
  0 & \ldots & 0 & 1 & \ldots & 1 \\
  a_1 & \ldots & a_n & a_{n+1} & \ldots & a_L
\end{pmatrix}.
\]

**Lemma 4.3.** Given a directed graph and bipartite graph as defined in Section 2. Assume that each connected component of the directed graph is strongly connected. There exists a set of values of the rate constants \( k_{ij} \) such that the following holds. For each set of positive values of the constants \( c_i \) in the conservation relations there exists a unique positive solution of \( I_{\tilde{A}} \Psi(x) = 0 \) and \( v^T_i x - c_i = 0, i = 1, \ldots, \).

**Proof.** Define \( z = I_{\tilde{A}} \Psi(x) \). If \( x \) is a positive solution of \( I_{\tilde{A}} \Psi(x) = 0 \) then \( z \in \ker(I_{\tilde{A}}) \cap (\mathbb{R}_+)^l \). That means we restrict Clarke’s cone to the polyhedral subcone generated by positive circuits of the directed graph. Let these positive circuits denote by \( E_i, i = 1, \ldots, c \). Then each \( z \in \ker(I_{\tilde{A}}) \cap (\mathbb{R}_+)^l \) is a convex combination of positive circuits, i.e., there exists \( j_i > 0 \) with \( z = \sum_{i=1}^{c} j_i E_i \).
To each connected component we can associate a set of monomials and a projective space. $z$ is a representative of a class in a product of these projective spaces. The polynomial system $I_u I_K \Psi (x) = 0$ is equivalent to a system consisting of special polynomials. Each polynomial has in its representation by monomials only monomials associated to one of the connected components. Consequently, we apply a modification of the Cayley trick.

For each connected component a slack variable $x_{-i}$, $i = 1, \ldots, s$, is introduced, where $s$ denotes the number of connected components. This corresponds to a lifting $\tilde{Y}_L \in \mathbb{Z}^{m+s}.$ in the following way. Each column of $Y_L$ is associated to a vertex $(\simeq \text{complex } \simeq \text{monomial})$ in one of the connected components. All columns of $Y_L$ associated to the $i$th connected component get a lifting with entry 1 in the $i$th row and zero otherwise. The multihomogeneous ideal $I_{\tilde{Y}_L} \subset \mathbb{C}[u]$ has a variety in the product of projective spaces. Analogously, there is the multihomogeneous deformed toric ideal $I_{\tilde{Y}_L}^{\text{def}} \subset \mathbb{C}(\mathbf{k})[z]$ is defined. If $[z] \in V(I_{\tilde{Y}_L}^{\text{def}})$ and $z \in \ker(I_u) \cap (\mathbb{R}^+)^l$ then there exists associated positive solutions $x$.

Since $z > 0$ it is sufficient to look at a lattice basis ideal

$$I_{\mathbf{C}}^{\text{def}} = \{ z^{g^+} - k \bar{g} z^-, \; g \text{ element of a module basis of } \ker(\tilde{Y}_L) \}.$$ 

By Lemma 12.2 in [34], $I_{\mathbf{C}}^{\text{def}} = (z_1 \cdots z_l)_{c_1}^{\infty} = \bar{I}_{\bar{Y}_L}$ and thus the positive parts of the varieties are equal, $V_+(I_{\tilde{Y}_L}^{\text{def}}) = V_+(I_{\mathbf{C}}^{\text{def}})$.

The columns of $Y_L$ consists of columns of $Y$. Some are repeated if the associated complex is an initial complex for several reactions. That means $I_{\mathbf{C}}^{\text{def}}$ includes linear polynomials. Since we demand $z = \sum_{i=1}^c j_i E_i \in V(I_{\mathbf{C}}^{\text{def}})$ there are linear conditions for the rate constants $k_{ij}$. But this only relates rate constants inside a connected component and coefficients $j_i$ of positive circuits of the same connected component. Besides this there is exactly one degree of freedom in $z$ for each connected component. This agrees with the fact that $I_{\tilde{Y}_L}$ is multihomogeneous. We complete the linear polynomials to a generating system of $I_{\tilde{Y}_L}^{\text{def}}$ by a module basis $g_1, \ldots, g_b$ of $\ker(\tilde{Y})$. This gives linear independent $\bar{Y}_1, \ldots, \bar{Y}_b \in \ker(\tilde{Y}_L)$ and thus independent parameters $k_{\bar{Y}1}, \ldots, k_{\bar{Y}b}$. Using $z \in V(I_{\tilde{Y}_L}^{\text{def}})$ again gives special values of the rate constants by solving $\bar{Y}_1 - k_{\bar{Y}1} z_1 = 0, \ldots, \bar{Y}_b - k_{\bar{Y}b} z_b = 0$ for the parameters. This proves the existence of positive solutions.

Whether there is one positive solution or infinitely many depends on the lattice associated to the Cayley trick which is the sum of the sublattices generated by the differences of the rate constants by solving $v_i^T x - c_i = 0,$ $i = 1, \ldots$ which implies uniqueness.

**Remark 4.4.**

(i) Lemma 4.3 contains the deficiency-zero-theorem in [15,21] as a subcase.

(ii) A positive solution $x$ which satisfies $I_u I_K \Psi (x) = 0$ as in the lemma above is called complex balancing [24]. This name is justified by their existence and uniqueness and the fact that they are asymptotically stable [6]. (iii) The complex balancing solutions are unique
as solutions of \( I_a I_k \Psi(x) = 0 \), \( v'_i x - c_i = 0 \) and unique as solutions of \( Y I_a \Psi(x) = 0 \), \( v'_i x - c_i = 0 \) which is shown in [24] using a Lyapunov function. (iv) In [24] a special subcase of complex balancing has another name. A solution \( x \) such that \( k_{ij} \Psi_j(x) = k_{ij} \Psi_i(x) \) for all forward–backward reactions \( C_i \leftrightarrow C_j \) is called detailed balancing. (v) In the complex balancing case the lattice associated to \( \hat{Y} \) is degenerate leading to free parameters. Two solutions \( a, c \) which just differ by values of this free parameters give rise to a vector \( \ln(a) - \ln(c) \) which is orthogonal to the lattice which generates a vector space equal to \( \text{im}(Y I_a) \). In [24] these two points are said to be quasi-thermostatic to each other.

In the proof a multiple lifting is introduced according to the connected components of the directed graph. We denote the multiple lifted matrices by \( \hat{Y} \) and \( \hat{Y}_L \) and \( \hat{Y}_e \). We call the polytope generated by the columns of \( \hat{Y}_L \), \( \text{Cayley-graph-polytope} \) in analogy to the Cayley polytope [22].

Now we turn the attention to various toric ideals. Besides the (multi)homogeneous toric ideals \( I \hat{Y} \), \( I \hat{Y}_L \), \( I \hat{Y}_e \), \( I \hat{Y}_L \), \( I \hat{Y}_e \) we are dealing with (multi)homogeneous deformed toric ideals \( I^{\text{def}} \hat{Y}_L \), \( I^{\text{def}} \hat{Y}_L \), \( I^{\text{def}} \hat{Y}_e \). For the latter \( t^{\text{def}} \hat{Y}_L \), \( t^{\text{def}} \hat{Y}_L \) we need to introduce dummy parameters for the rate constants of pure product complexes.

\( I \hat{Y}_e \) is related to minimal generators of Clarke’s cone which are not positive circuits of the directed graph. If \( \text{rank}(Y I_a) < \text{rank}(I_a) \) then such stoichiometric generators exist obviously. Each stoichiometric generator \( E_i \) of \( \text{ker}(Y I_a) \cap (\mathbb{R}_{>0})^s \) yields a non-zero vector \( I_a E_i \). By suitable rescaling the vector has integer entries which are coprime. Our notation is \( g_i = \text{normalize}(I_a E_i) \). Following [16] we call \( g_i \) confluent vector. Let \( s \) be the number of stoichiometric generators. Of course \( g_1, \ldots, g_s \) may be linear dependent.

**Lemma 4.5.** Given the directed graph and bipartite graph with matrices \( Y_r \), \( Y_L \), \( Y_e \), \( Y = Y_s = Y_k \) as in Section 2 we denote by \( \hat{Y} \) the lifting induced by the connected components of the directed graph.

(i) The confluent vectors \( g_1, \ldots, g_s \) generate the nullspace of \( \hat{Y} \) as a vector space.

(ii) The toric ideal \( I \hat{Y} \) is multihomogeneous and contains binomials \( w^{k_i^+} - w^{k_i^-} \), \( i = 1, \ldots, s \). Moreover,

\[
I \hat{Y} = \langle w^{k_1^+} - w^{k_1^-}, \ldots, w^{k_s^+} - w^{k_s^-} \rangle : \langle w_1 \cdots w_n \rangle^\infty.
\]

(iii) Let \( \mathcal{G} \) be a renumbering and filling with zeros of \( g_i \) such that \( \mathcal{G}_i \in \ker(\hat{Y}_e) \) for \( i = 1, \ldots, s \). Let \( I_D \) be the ideal generated by \( z^{k_i^+} - z^{k_i^-} \), \( i = 1, \ldots, s \), and all linear polynomials \( z_i - z_j \) corresponding to multiple initial complexes. Then

\[
I \hat{Y}_e = I_D : \langle z_1 \cdots z_d \rangle^\infty,
\]

where \( d \) is the number of columns of \( Y_e \).

**Proof.** Since \( \ker(Y I_a) = \ker(I_a) \oplus \text{span}(E_1, \ldots, E_s) \) we have \( \text{span}(g_1, \ldots, g_s) \subseteq \ker(Y) \). In fact \( \text{span}(g_1, \ldots, g_s) \subseteq \ker(Y) \) because \( \ker(Y) \subseteq \text{im}(I_a) \) since the lifting \( \hat{Y} \) of \( Y \) is
induced by the directed graph. But $I_\alpha$ restricted to a complement of $\ker(I_\alpha)$ is invertible. Thus $(I_\alpha)^{-1}(\ker(Y)) \subseteq \ker(Y I_\alpha)$. Consequently, $g_1, \ldots, g_\upsilon$ generate $\ker(Y)$. (ii) follows from (i) and Lemmas 4.1 and 12.2 in [34]. (iii) follows from elementary linear algebra and [34] again. □

**Remark 4.6.** (i) For deficiency one $\dim(\ker(Y)) = 1$ and its generator $g_1$ is a circuit of $Y$. (ii) If the directed graph has connected components which are all strongly connected then $Y_\ell = Y_e$ and Lemma 4.5(iii) gives $I^{\text{def}}_{\ell e} = I^{\text{def}}_D : (z_1 \cdots z_\upsilon)^\infty$.

In view of the Cayley trick we refine the new rate constants $k^{\text{new}} = (k_{0, \hat{\ell}, \hat{c})}$. We consider the case that no complexes are pure product complexes which includes the case of Lemma 4.3 where all connected components of the directed graph are strongly connected. If the lattice generated by $y_2 - y_1, \ldots, y_n - y_1$ has larger rank than the lattice associated to the Cayley-graph-polytope (which is generated by differences inside connected components) then we subdivide both tuples $\hat{c}$ and $\hat{\ell}$.

It is possible to choose toric rate constants $\hat{k}_1^c, \ldots, \hat{k}_c^c$ associated to the lattice of the Cayley-graph-polytope (with dimension $c$) and complete them to a full set of toric rate constants $\hat{k}_c+1, \ldots, \hat{k}_R$ corresponding to the lattice.

Obviously, $I_{\hat{c}} \subseteq I_{\hat{c}}$ in $C[w_1, \ldots, w_\upsilon]$ and thus $I^{\text{def}}_{\hat{c} \hat{c}} \subseteq I^{\text{def}}_C$. With the help of Lemma 4.5 we subdivide the tuple $\hat{c}$. For a pair of reactions $C_i \rightarrow C_j$ and $C_i \rightarrow C_v$ we choose $k_{ijv} = k_{jj}/k_{ij}$. From the confluent vectors we choose a maximal linear independent set $g_1, \ldots, g_l$ and choose

$$k_{g_i} = \hat{k}^{\bar{g}_i} = \prod_{C_{j} \leftarrow C_{\mu}} (k_{\mu \nu})^{(\bar{g}_i)}_{(\bar{g}_i)}, \quad i = 1, \ldots, t,$$

(11)

as parameters. We refer to them as confluent rate constants. The $k_{g_i}$ and $k_{ijv}$ are clearly some independent representatives of $C^{l-1}/C^R$. Some binomial generators in $I^{\text{def}}_C$ which are not in $I^{\text{def}}_C$ give the remaining new rate constants.

Now we are ready to present an example for Lemma 4.3.

**Example 4.7.** This example is due to Edelstein and has been investigated before by Feinberg and in [21]. The reactions are

$$C_1 \xleftrightarrow{k_{1,2}} C_2, \quad C_3 \xleftrightarrow{k_{3,4}} C_4 \xleftrightarrow{k_{4,5}} C_5$$

with stoichiometric matrix

$$Y = \begin{pmatrix} 1 & 2 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad \text{yielding} \quad 0 = -k_{4,3}x_1x_2 + (k_{3,4} + k_{5,4})x_3 - k_{4,5}x_2,$$

$$0 = k_{4,5}x_1x_2 + (-k_{3,4} - k_{5,4})x_3 + k_{4,5}x_2.$$
Then $g_4 := I_a E_4 = (-1, 1, -1, 0, 1)$ and $I_a E_5 = -g_4$. The confluent vector gives the Groebner basis of $I_a = \langle w^{z_1} - w^{z_2} \rangle = \langle w_2 w_5 - w_1 w_3 \rangle$. All complexes are reaction complexes, but the fourth complex gives rise to two reactions. Thus the deformed toric variety contains a linear relation. The two homogeneous toric ideals $I_{4_a}$ and $I_{5_a}$ are equal and thus

$$I_{4_a}^{\text{def}} = I_{5_a}^{\text{def}} = \langle z_4 k_{5,4} - z_5 k_{3,4}, z_6 z_2 k_{4,3} - z_1 z_3 k_{4,5} k_{1,2} \rangle.$$ 

This suggests to use $\tilde{k}_{435} = \frac{k_{435}}{k_{5,4}} = \frac{k_{43}}{k_{5,3}} = \frac{k_{4}}{k_{3,3}}$ and $k_{43} = \frac{k_4}{k_{3,3}}$ as new parameters (toric rate constants), where $\tilde{k} = (k_{2,1}, k_{1,2}, k_{4,3}, k_{3,4}, k_{4,3}, k_{4,5})$ and $e_{45} = (0, 0, 0, 1, -1, 0)$ and $\tilde{g}_4 = (-1, 1, -1, 0, 0, 1)$. They can be read off from the Cayley trick. Each $[z] \in \mathbb{P}^1 \times \mathbb{P}^3$ which is in $V(I_{4_a}^{\text{def}})$ such that $z$ is in the cone generated by $E_1, E_2, E_3$ gives rise to complex balancing solutions by solving

$$z_1 = k_{2,1} x_0 x_1, \quad z_2 = k_{1,2} x_1, \quad z_3 = k_{4,3} x_1 x_2, \quad z_4 = k_{3,4} x_3, \quad z_5 = k_{5,4} x_3, \quad z_6 = \frac{k_{4,5} z_1}{k_{4,3} z_1},$$

(12)

Only Eqs. (12) are important for the Cayley trick. They suggest the change of coordinates $x_1 = u_1$, $x_2 = u_3$, $x_3 = w_2 w_3$ or equivalently $u_1 = x_1$, $u_2 = x_3/(x_1 x_2)$, $u_3 = x_2$. That means Eqs. (12) determine $u_1$, $u_2$ and leave $u_3$ arbitrary. The lattice associated to the Cayley trick has dimension two while the whole lattice has dimension three. So the new coordinates are $k_{\text{new}} = (k_0, \tilde{k}_{2,1}, \tilde{k}_{4,3}, k_3, k_{435}, k_{5,4})$. The ansatz for a change of coordinates with $B$ and $C$ gives an affine linear space of solutions of dimension 8. We choose

$$k_{2,1} = \frac{k_0}{k_{2,1}}, \quad k_{1,2} = \frac{k_0 \tilde{k}_C}{k_{2,1}}, \quad k_{4,3} = \frac{k_0 \tilde{k}_C}{k_{2,1}}$$

or equivalently

$$k_0 = \frac{k_{2,1} k_{3,4}}{k_{4,3}}, \quad \tilde{k}_{2,1} = \frac{k_{1,2}}{k_{2,1}}, \quad \tilde{k}_{4,3} = \frac{k_{4,3}}{k_{3,4}}, \quad \tilde{k}_3 = \frac{k_{4,3}}{k_{2,1}}.$$

Then

$$I_{4_a}^{\text{def}} = \langle z_4 - \tilde{k}_{435} z_5, z_6 z_2 - k_{5,4} z_1 \rangle.$$
The toric variety is independent of $\tilde{k}_1^C, k_2^C, \tilde{k}_3$ which are the rescalings of $k_{ij}$ inherited from the torus action on $x$. For each $z \in V(I_{Y_L}^{\text{def}}) \subset \mathbb{P}^1 \times \mathbb{P}^3$ we need to solve $z_2/z_1 = \tilde{k}_1^C w_1$ and $z_4/z_3 = \tilde{k}_2^C w_2$ from (12). Remember for complex balancing solutions $z = \sum_{i=1}^5 j_i E_i$ with $j_4 = j_5 = 0$ or equivalently $z_1 = z_2$, $z_3 = z_4$, $z_5 = z_6$. Then $z \in V(I_{Y_L}^{\text{def}})$ implies $\hat{k}_{435} = j_2/j_3$ and $k_{g_4}\hat{k}_{435} = 1$. This gives the family of complex balancing solutions

$$x = \left( \frac{1}{\hat{k}_1^C}, w_3, \frac{w_3}{\hat{k}_1^C \hat{k}_2^C} \right)$$

which is obviously transversal to the affine spaces $\{x \mid x_2 + x_3 - c_1 = 0\}$ in $(\mathbb{R}_+)^3$. Observe that the complex balancing solutions are independent of $\hat{k}_3$.

We still need to discuss how we change coordinates for the case that the directed graph has pure product complexes. For each pure product complex $C_i$ we suggest to introduce a slack constant $k_{i,i}$. Instead of studying the intersection of Clarke’s cone with $V(I_{Y_L}^{\text{def}})$ we amend the cone by new coordinates $z_{i+j}$. Then we intersect Clarke’s cone with the variety of $I_{Y_L}^{\text{def}}$. Since the confluent vectors $g_i$ give rise to vectors $\bar{g}_i \in \ker(\tilde{Y}_r)$ we can still use the confluent rate constants $k_{g_i}$. Eventually, the number of toric rate constants increases. Only choices of new rate constants $k_{\text{new}}$ are relevant which corresponds to $k_{i,i} = 0$ for all pure product complexes. An example will be given below.

Before describing the transition to the limit we start with the situation arising in the limit itself.

**Proposition 4.8.** Assume a system (5) with mass action kinetics such that the following conditions are satisfied.

(i) The directed graph is a forest of trees and each connected component contains only one strong connected component (here a sink).

(ii) The system has deficiency one: $\text{rank}(Y_{I_a}) - \text{rank}(I_a) - 1$ and there exists a generator $E \in (\mathbb{R}_+)^l$ of $\ker(Y_{I_a})$ which is positive.

(iii) $\tilde{Y}_r$ has maximal rank $r$, the number of reactant complexes.

Then there exist values of the constants $c_i$ in the conservation relations such that the space $\{x \in \mathbb{R}_+^l \mid v_i^T x - c_i = 0, i = 1, \ldots, m - \text{rank}(Y_{I_a})\}$ contains at least one positive solution of $Y_{I_a} I_K \Psi(x) = 0$. If $r < m$ then the real positive variety of $Y_{I_a} I_K \Psi(x) = 0$ has higher dimension and is parameterized by $m - r$ parameters. Assume the directed graph consists of more than one connected component and $y_1, \ldots, y_r$ are the columns of $Y$ corresponding to reaction complexes. Assume there exists a vector $\mu \in \text{span}(y_2 - y_1, \ldots, y_r - y_1)$ such that

(iv) The vector $\mu$ is not orthogonal to $\text{im}(Y_{I_a})$.

(v) There exists a positive solution $x$ of $Y_{I_a} I_K \Psi(x) = 0$ such that $\text{diag}(x)\mu \in \text{im}(Y_{I_a})$. 
Then in a generic situation there exist positive values for $c_i$ such that $\{ x \in \mathbb{R}^l_+ \mid v^i_1 x - c_i = 0, i = 1, \ldots \}$ contains at least two positive solutions of the system $Y_L I_K \Psi(x) = 0$.

**Proof.** We study the intersection of the convex polyhedral cone $\text{ker}(Y_L) \cap (\mathbb{R}_{\leq 0})^l$ with the deformed toric variety $V(I_{\tilde{Y}_{r}}^\text{def})$. By (i) there are no minimal generators of the cone which are positive circuits of the directed graph. By (ii) the cone is generated by one stoichiometric generator $E$. In order to solve $E = I_K \Psi(x) x_0$ we observe that $\text{rank}(I_L) = \text{rank}(I_L I_K)$ if each connected component contains just one strong connected component. By (i) this guarantees that $E = I_K \Psi(x) x_0$ is equivalent to a binomial system $x_0 x^{y_1} = b_1, \ldots, x_0 x^{y_r} = b_r$ where the $y_1, \ldots, y_r$ correspond to reactant complexes and the $b_i$ are positive numbers depending on the values of $k_{ij}$ and the components of $E$. The toric variety $V(I_{\tilde{Y}_{r}})$ is equivalent to the projective space $\mathbb{P}^{r-1}$ by (iii). Solving the binomial system by Hermite normal form $U \tilde{Y}_r = H$ we introduce new coordinates

$$x_0 = u^{(0)}_0 \cdots u^{(0)}_m, \ldots, x_m = u^{(m)}_0 \cdots u^{(m)}_m,$$

(13)

where $U = (a_{ij})_{i,j=0,\ldots,m}$ is unimodular. For the first set of new coordinates $w_1, \ldots, w_r$ there is precisely one positive solution of the binomial system. The coordinates $w_{r+1}, \ldots, w_m$ not appearing in the system parameterize the variety. Choosing for these coordinates values equal to 1 and substituting $x = x(w)$ into the conservation relations we find values for $c_i$. If $m > r$, then there exist unrestricted variables $w_i$, $i = r+1, \ldots, m$. In (13) the submatrix $U^r = (a_{ij})_{j=1,\ldots,r,i=r+1,\ldots,m}$ determines the dependence on $w_{r+1}, \ldots, w_m$. The rows $\mu_i = \text{row}_i(U^r)$ are orthogonal to the lattice $y_2 - y_1, \ldots, y_r - y_1$ and define a tangent to the variety, i.e.,

$$\frac{dx}{dw_i} = \text{diag}(x) \mu_i \frac{1}{w_i}, \quad i = r+1, \ldots, m.$$

If for some particular values of $w_{r+1}, \ldots, w_m$ and $\mu = \sum_{i=r+1}^m \mu_i(1/w_i)$ the vector $\text{diag}(x(w_{r+1}, \ldots, w_m)) \mu$ is an element of $\text{im}(Y_L)$ then the variety is touching the space $\{ x \mid v^i_1 x - c_i, i = 1, \ldots \}$ for special values of $c_i$. This happens if $m - r \geq m - \text{rank}(Y_L)$ and there is a $\mu \in \text{span}(\mu_{r+1}, \ldots, \mu_m) = \text{span}(y_2 - y_1, \ldots, y_r - y_1)$ which is not orthogonal to $\text{im}(Y_L)$ (condition (iv)) and $\text{diag}(x)$ is rescaling $\mu$ to an element of $\text{im}(Y_L)$ (condition (v)). Condition (iv) is necessary for condition (v). Under a genericity condition on higher derivatives there is multistationarity. □

**Remark 4.9.** A variation of the lemma still states the existence of a solution. There (i) is weakened to the structure of a forest of trees only. To (ii) we add: for each pair of arrows $C_j \rightarrow C_i, C_j \rightarrow C_p$ with indices $\mu, \nu$ the stoichiometric generator satisfies $k_{ij} E_{\nu} - k_{pj} E_{\mu} = 0$.

**Example 3.11 (continued).** We consider the subsystem given by the stoichiometric generator $E_3 = (0, 1, 0, 1, 1)$. The directed graph is

$$C_1 \xrightarrow{k_{1,2}} C_2 \quad \xrightarrow{k_{3,4}} C_3 \quad \xleftarrow{k_{3,4}} C_4 \quad \xrightarrow{k_{5,5}} C_5.$$

Then the polynomial subsystem is

\[
\begin{align*}
0 &= k_1 x_1^2 - k_{6,5} x_1 x_2, \\
0 &= k_3 x_3 - k_{6,5} x_1 x_2, \\
0 &= -2k_1 x_1^2 - k_{3,4} x_3 + 3k_{6,5} x_1 x_2, \\
0 &= 2x_1 + x_2 + x_3 - c_1
\end{align*}
\]

with \( Y_r = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 2 & 1 & 0 \end{pmatrix} \) and \( E = (1, 1, 1) \).

A solution is given by intersecting the nullspace of the coefficient matrix (here span(\(E\))) with the homogeneous toric variety which is \( \mathbb{P}^2 \). Solving \( k_1 x_0 x_2^2 = 1 \), and \( k_{3,4} x_0 x_1 = 1 \) and \( k_{6,5} x_0 x_1 x_2 = 1 \) yields

\[
(x_1, x_2, x_3) = \left( \frac{k_{3,4}}{k_{1,2} k_{6,5} w}, w, \frac{k_{3,4}}{k_{1,2}} \right),
\]

where \( w \) is an arbitrary number, since the lattice is degenerate.

For \( w = k_{3,4} \sqrt{2}/\sqrt{k_{1,2} k_{6,5}} \) the tangent to the curve \( \frac{dx}{d\omega} = (-1/2, 1, 0) \in \text{im}(Y_{I_0}) \) is orthogonal to the conservation vector \( v_1 \). For

\[
c_1 = \frac{(k_{6,5} + \sqrt{2} \sqrt{k_{1,2} k_{6,5}}) k_{3,4}}{k_{1,2} k_{6,5}}
\]

the curve is touching the space \( \{ x \in \mathbb{R}^3_+ \mid 2x_1 + x_2 + x_3 = c_1 \} \), while for larger values of \( c_1 \) the curve intersects in two positive solutions \( x, \tilde{x} \) corresponding to \( w \) and \( \tilde{w} \). Then

\[
\mu = (\ln(x_1/\tilde{x}_1), \ln(x_2/\tilde{x}_2), \ln(x_3/\tilde{x}_3)) = \ln \left( w/\tilde{w} \right) \cdot (-1, 1, 0),
\]

may be defined which is not parallel to \( v_1 \), but orthogonal to the Newton polytope generated by \( y_2, y_4, y_5 \), see Fig. 10.

In order to study multistationarity we need more definitions.

**Definition 4.10** [34]. Given \( A = (a_1, \ldots, a_n) \subset \mathbb{R}^{m,n} \) of rank \( m \). A triangulation \( \Delta \) of conv(\(a_1, \ldots, a_n\)) is a set of \( m \)-simplices \( S_i = \{a_{i0}, \ldots, a_{in}\} \) such that conv(\(a_1, \ldots, a_n\)) = \( \bigcup_i \text{conv}(S_i) \) and conv(\(S_i\)) \( \cap \text{conv}(S_j) = \text{conv}(S_i \cap S_j), \forall i \neq j \). A triangulation is called regular and denoted \( \Delta_{\omega} \) if it is induced by a lifting, i.e., there are values \( \omega_1, \ldots, \omega_n \) such that conv(\(S_i\)) are the projected lower facets of conv(\(A^\omega\)) where

\[
A^\omega = \begin{pmatrix} \omega_1 & \cdots & \omega_n \\ a_1 & \cdots & a_n \end{pmatrix}.
\]

**Definition 4.11** [34]. For a triangulation \( \Delta \) of \( a_1, \ldots, a_n \) the Stanley–Reisner ideal is defined as

\[
I_\Delta = \left\{ \prod_{j \in \sigma} z_j \mid \sigma \subset \{1, \ldots, n\} \text{ such that } a_j, j \in \sigma \text{ do not form a face of } \Delta \right\}.
\]
Recall that for a given ideal $I \subseteq k[x_1, \ldots, x_n]$ almost all term orders can be represented by a vector $\omega \in \mathbb{R}^n$. Given an ideal, all term orders $\omega \in \mathbb{R}^n$ with the same reduced Gröbner basis form a cone. There are finitely many cones forming the Gröbner fan. A result in [34] states that each reduced Gröbner basis of $I_A$ yields a regular triangulation. Moreover, $\sqrt{\text{in}(I_A)} = I_\triangle$ for a term order and lifting $\omega$. Circuits of $\hat{A}$ are important since they distinguish two regular triangulations. All lifting vectors $\omega$ of $\bar{A}$ giving the same regular triangulation form a cone. The set of these cones is the secondary fan. The Gröbner fan of a toric ideal $I_\hat{A}$ is a refinement of the secondary fan. More about this can be found in [34, Chapters 1–3, 8], [3,22,31].

Now we will be interested in regular triangulations of the Cayley-graph-polytope, of the Newton polytope as well as of the polytope which is the convex hull of the columns of $YL$, or of $Ye$.

The Gröbner fans of toric ideals are special. Since $I_A$ is weighted homogeneous with respect to each row we can restrict to consider term orders $\omega \in \ker(A)$.

**Lemma 4.12.** Assume a vector space basis of $\ker(\bar{Y})$ is given by confluent vectors $g_1, \ldots, g_t$. Each term order of $I_{\bar{Y}}$ is represented by a vector $\omega = \omega_1g_1 + \cdots + \omega_tg_t$. There exists a vector of signs $v_1, \ldots, v_t \in \{+, -\}$ and a regular triangulation $\triangle$ of $\bar{Y}$ such that

$$\langle w^{\gamma_1}, \ldots, w^{\gamma_t} \rangle \subseteq \text{in}_{\omega}(I_{\bar{Y}}) \quad \text{and} \quad \sqrt{\text{in}_{\omega}(I_{\bar{Y}})} = I_{\triangle}$$

with $\gamma_1 = g^{v_1}, \ldots, \gamma_s = g^{v_s}$ being the positive or negative parts of the confluent vectors. In particular, there exists a term order $\omega$ with $\langle w^{\gamma_1}, \ldots, w^{\gamma_t} \rangle \subseteq \text{in}_{\omega}(I_{\bar{Y}})$.

**Proof.** Since toric ideals are multihomogeneous we may restrict to vectors $\omega \in \ker(\bar{Y}) = \text{span}(g_1, \ldots, g_t)$ to represent term orders. For each confluent vector $g_i$, the polynomial $w^{g_i} - w^{-g_i}$ is an element of $I_{\bar{Y}}$, by Lemma 4.5. If $\omega'g_i^+ > \omega'g_i^-$ then $lt(w^{g_i^+} - w^{g_i^-}) = w^{g_i^+}$ and thus $w^{g_i^+} \in \text{in}_{\omega}(I_{\bar{Y}})$ else $w^{g_i^-} \in \text{in}_{\omega}(I_{\bar{Y}})$. The existence of the regular triangulation follows from [34]. □

Each confluent vector $g_i$ defines a hyperplane $\{ w \in \mathbb{R}^n | w^j g_i = 0 \}$ which divides the space $\mathbb{R}^n$ into halfspaces. The intersections of all these halfspaces are convex polyhedral cones which form a fan. The lemma above states that the Gröbner fan of $I_{\bar{Y}}$ is a refinement of this fan.

In general the confluent vectors $g_i$ are not primitive and thus the associated binomials are in general not elements of the universal Gröbner basis.

**Lemma 4.13.** Assume a vector space basis of $\ker(\bar{Y})$ is given by confluent vectors $g_1, \ldots, g_t$. The associated elements of $\ker(\bar{Y}_e)$ are denoted by $\bar{g}_1, \ldots, \bar{g}_t$ and completed by differences $e_{ij} = e_i - e_j$ of unit vectors to form a vector space basis of $\ker(\bar{Y}_e)$. For each

$$\omega = \omega_1\bar{g}_1 + \cdots + \omega_t\bar{g}_t + \sum_{C_k \to C_\alpha, C_k \to C_\mu} \omega_{ij} e_{ij},$$

where...
representing a term order for $I_{\tilde{Y}_e}$, the following holds.

(i) For $i = 1, \ldots, s$ there is a sign $v$ such that $w_{\bar{g}^+_i} \in \text{in}_\omega(I_{\tilde{Ye}})$.

(ii) For each pair of reactions $C_k \overset{i}{\rightarrow} C_v, C_k \overset{j}{\rightarrow} C_\mu$ either $w_i \in \text{in}_\omega(I_{\tilde{Ye}})$ or $w_j \in \text{in}_\omega(I_{\tilde{Ye}})$.

(iii) There exists a regular triangulation $\tilde{\Delta}$ of $\tilde{Y}_e$ such that its Stanley–Reisner ideal $I_{\tilde{\Delta}}$ is the radical of the initial ideal $\text{in}_\omega(I_{\tilde{Ye}})$.

**Proof.** This is a corollary of the previous lemma since the columns of $Y$ and $Ye$ are equal besides that in $Ye$ some columns are repeated if a complex is the initial complex for several reactions. □

The term order $\omega = \sum_{i=1}^t \omega_i \bar{g}_i$ is also a lifting vector. If $\omega = \bar{g}_i$ is generic, then the lifting defines a regular triangulation, otherwise it defines a cell complex.

**Lemma 4.14.** Let $g_1, \ldots, g_t$ denote the confluent vectors. Then for $i = 1, \ldots, s$:

(i) The cell complex of $\tilde{Y}$ associated to $g_i$ includes a face given by $\text{supp}(g_i^-)$.

(ii) The cell complex of $\tilde{Ye}$ associated to $\bar{g}_i$ in includes a face given by $\text{supp}(\bar{g}_i^-)$.

**Proof.** The lifting of $y_j$ is zero, if $j \in \text{supp}(g_i)$. It is positive, if $j \in \text{supp}(g_i^+)$, and negative for $j \in \text{supp}(g_i^-)$. Since the cardinality of $\text{supp}(g_i^-)$ is less than or equal to the rank of $\tilde{Y}$, the lifted vector $y_j, j \in \text{supp}(g_i^-)$, generates a face of the lower hull of the polytope generated by $\tilde{Y}_e$. By projection this gives a face of the regular triangulation which proves (i). Analogously, (ii) is proved. □

Of course, regular triangulations/cell complexes defined by lifting vectors sufficiently close to $g_i$, still have the face associated to $\text{supp}(g_i^-)$. The lemma shows that each confluent vector $g_i$ is a representative of a cone in the secondary fan of $\tilde{Y}$. If $\text{in}_\omega(I_{\tilde{Ye}}^{\text{def}})$ is square-free, then we know more about the regular triangulation $\tilde{\Delta}_\omega$. For $j = 1, \ldots, s$ the following holds. If $g_j^+ \in \text{in}_\omega(I_{\tilde{Ye}}^{\text{def}})$, then $\text{supp}(g_j^-)$ defines a face of $\tilde{\Delta}_\omega$. If $g_j^- \in \text{in}_\omega(I_{\tilde{Ye}}^{\text{def}})$, then $\text{supp}(g_j^+)$ defines a face.

For each cone in the Gröbner fan we investigate a toric deformation.

**Proposition 4.15.** Assume a term order $\omega \in \mathbb{R}^d$ for $I_{\tilde{Ye}}^{\text{def}}$ which is a linear combination of $\bar{g}_1, \ldots, \bar{g}_t, e_{ij}$ and assume the matrix $B$ of the change of rate constants (10). The components of $\Omega = (B^t)^{-1}\omega$ corresponding to $\bar{g}_i, e_{ij}$ are denoted by $\omega_i, \omega_{ij}$. Then the one-parameter family of new rate constants $k_{\bar{g}_i} = \epsilon^{\omega_i}, i = 1, \ldots, t$, $\hat{k}_{k_{\nu \mu}} = \epsilon^{\omega_{ij}}$ for $C_k \overset{i}{\rightarrow} C_v, C_k \overset{j}{\rightarrow} C_\mu$ defines a flat deformation from $I_{\tilde{Ye}}^{\text{def}}$ to the monomial ideal $\text{in}_\omega(I_{\tilde{Ye}}^{\text{def}})$.
Proof. Each \( \omega \) which represents a term order gives a reduced Gröbner basis of \( I_{\hat{Y}_e} \) which consists of binomials in \( Q(\hat{k}_{k\nu\mu}, k_{gi})[z] \), since the ideal is toric. Each element in the reduced Gröbner basis is of the form

\[
\frac{z^{\alpha^+} - k^\alpha z^{\alpha^-}}{c_\nu, c_{\mu-i}} = \left( \prod_{i=1}^t (\hat{k}_{k\nu\mu})^{\alpha_{ij}} \prod_{i=1}^t k_{gi} \right) z^{\alpha^-}
\]

with \( \alpha \in \ker(\hat{Y}_e) = \text{span}(e_{ij}, \bar{g}_1, \ldots, \bar{g}_t) \) and thus \( \alpha = Ca = \sum_{ij} \alpha_{ij} e_{ij} + \sum_{i=1}^t \alpha_i \bar{g}_i \). The special choice of a one-parameter family gives

\[
\frac{z^{\alpha^+} - \varepsilon^d \alpha z^{\alpha^-}}{c_\nu, c_{\mu-i}}
\]

because \( \sum_i \alpha_i \omega_i + \sum_{ij} \alpha_{ij} \omega_{ij} = \alpha' \Omega = (B\alpha)'(B')^{-1} \omega = \alpha' \omega \). On the other hand, we know that \( z^{\alpha^+} \) is the leading term and thus \( \omega' \alpha > 0 \). Then \( \lim_{\varepsilon \to 0} \left( \frac{z^{\alpha^+} - \varepsilon^d \alpha z^{\alpha^-}}{c_\nu, c_{\mu-i}} \right) = z^{\alpha^+} \).

This proves the deformation to the leading monomial ideal. \( \square \)

Lemma 4.16. The projective variety \( V(\text{in}_{\omega}(I_{\hat{Y}_e}^{\text{def}})) \subseteq \mathbb{P}^{d-1} \) is a collection of projective subvarieties which are isomorphic to projective spaces (of dimension \( \text{rank}(\hat{Y}) - \# \text{components} - 1 \)). For each subvariety there is a simplex in the associated regular triangulation \( \Delta_{\omega} \) of \( \hat{Y}_e \) and vice versa. For each projective subvariety the intersection with the (amended) Clarke’s cone \( \text{cone}(E_1, \ldots) \) is a subcone generated by some of the minimal generators \( E_i \).

The subcones define non-negative solutions of system (5) in a general way. Each projective space corresponds to a subcone and it corresponds to a subsystem of (5), since components of \( z \) are zero.

This is a generalization of Viro’s method. In the original Viro method a homotopy parameter \( t \) is artificially introduced. The limit \( t \to 0 \) deforms the homogeneous toric variety into projective spaces. This also defines a regular triangulation with a subsystem for each simplex. The solutions of the subsystems are deformed to solutions of the original system [22,32,33,35].

Definition 4.17. For a simplex in a regular triangulation \( \tilde{\Delta} \) we define a subsystem of \( Y I_a I_K \Psi(x) = 0 \) in the following way. Denote the columns of \( Y I_a \) by \( (Y I_a)_j \), \( j = 1, \ldots, d \). For the set of indices \( J \subseteq \{1, \ldots, d\} \) of a simplex we define

\[
\sum_{j \in J} (Y I_a)_j (I_K \Psi(x))_j
\]

and perform the change of coordinates (10) and substitute \( k_{gi} = 1 \) and \( \hat{k}_{ij\nu} = 1 \) for all \( i, j \).

Theorem 4.18. Assume the setting above, in particular the flat deformation, the regular triangulation \( \tilde{\Delta} \) of \( \hat{Y}_e \) and the subsystems associated to the simplices of \( \tilde{\Delta} \). The set \( \{x \in \mathbb{P}^{d-1} \} \)
(\mathbb{R}_{\geq 0})^m \mid \vhat{k}_j > 0 \text{ with } Y I_x I_x \Psi (x) = 0 \text{ deforms by } \varepsilon \to 0 \text{ via the flat deformation to the generalized solutions of the subsystems for all } \vhat{k}_j > 0. \text{ In particular, for fixed values of } \vhat{k}_j, \vhat{k}_{j+1}, \ldots, \vhat{k}_R \text{ the intersection with spaces } \{ x \mid v^i x - c_i = 0, i = 1, \ldots \} \text{ deforms to generalized solutions of the subsystems which also satisfy the conservation relations } v^i x - c_i = 0, i = 1, \ldots. $

Observe that finding the positive solutions of a subsystem is related to Clarke's cone. The positive solutions of a subsystem of a simplex with index set $J$ can be restricted to span those minimal generators $E_i$ with $\text{supp}(E_i) \subseteq J$. If we use coordinates $w$ associated to the lattices (instead of $x$) and keep $\vhat{k}_j$ arbitrary, then we only determine some of the $w_i$, namely those which are associated to the lattice of the Cayley-graph-polytope.

When one solves for positive solutions for fixed values of $k_j, k_{j+1}, \ldots, k_R$ one still needs to consider the ideal $I_{\vhat{Y}_e}$ additional to $I_{\vhat{Y}_e} = I_{\vhat{Y}_e}$ as in Theorem 4.18. If a cell of a regular triangulation of $\vhat{Y}_e$ shows multistationarity, then there is multistationarity for small $\varepsilon$ by continuity.

**Example 4.7 (continued).** Since $C_4$ is an initial complex for two reactions the matrix $Y = (y_1, y_2, y_3, y_4, y_5)$ is expanded to $Y_e = Y_L = (y_1, y_2, y_3, y_4, y_5)$. Term orders of

$$I_{\vhat{Y}_e} = I_{\vhat{Y}_e} = I_{\vhat{Y}_e} = (z_4 - \vhat{k}_4 z_5, z_6 z_2 - k_{g_4} z_1 z_3)$$

can be restricted to span$(e_{45}, \vhat{g}_4)$. There are four different reduced Gröbner bases.

1. For $\omega = e_{45} + \vhat{g}_4$ we deform the toric ideal with $\vhat{k}_{435} = \varepsilon, k_{g_4} = \varepsilon$ and $\varepsilon \to 0$ to $(z_4, z_6 z_2) = (z_2, z_4) \cap (z_4, z_6)$. This corresponds to a regular triangulation with simplices $\{z_1, z_3, z_5, z_6\}$ and $\{z_1, z_2, z_3, z_5\}$. The intersections of the two subvarieties $V((z_2, z_4)), V((z_4, z_6))$ with Clarke's cone are the boundary subcones cone$(E_3, E_4)$ and cone$(E_1, E_4)$.

2. For $\omega = -e_{45} - \vhat{g}_4$ we deform the toric ideal with $\vhat{k}_{435} = \varepsilon^{-1}, k_{g_4} = \varepsilon^{-1}$ and $\varepsilon \to 0$ to $(z_5, z_1 z_3) = (z_1, z_3) \cap (z_3, z_5)$. This corresponds to a regular triangulation with simplices $\{z_2, z_3, z_4, z_6\}$ and $\{z_1, z_2, z_4, z_6\}$. The intersections of the two subvarieties with Clarke's cone are the boundary subcones cone$(E_1, E_3)$ and cone$(E_2, E_3)$.

3. For $\omega = e_{45} - \vhat{g}_4$ the deformation gives $(z_4, z_1 z_3) = (z_1, z_4) \cap (z_3, z_4)$. The subcones are generated by $E_3$ and by $E_1, E_3$, respectively.

4. For $\omega = -e_{45} + \vhat{g}_4$ the deformation gives $(z_5, z_2 z_6) = (z_2, z_5) \cap (z_5, z_6)$. The subcones are generated by $E_2$, as well as by $E_1, E_2$.

The cases (3) and (4) are the two extreme subcases of the case of complex balancing solutions studied before.

The cases (1) and (2) use the regular triangulations of the Cayley-graph-polytope of $\vhat{Y}_e$. In this example the projections of the two regular triangulations of $\vhat{Y}_e$ give regular triangulations of the Newton polytope conv$(y_1, \ldots, y_5)$ which are presented in Fig. 7. The inner face $\{z_1, z_3, z_5\}$ of the first triangulation corresponds to the support of $E_4$ and includes the support of $\vhat{g}_4$. The inner face $\{z_2, z_4, z_6\}$ of the second triangulation corresponds to
the support of $E_5$ and includes the support of $\overline{E}_5$. The inner normal of the first inner face is $\mu = (1, 0, 1)$. For the second it is $\mu = (1, 2, 2)$. Both normals are not parallel to $v_1 = (0, 1, 1)$. But condition (v) of Proposition 4.8 is not satisfied. There is no multistationarity for the stoichiometric subsystems. Nevertheless there is multistationarity in the limit of case (1).

The set \( \{ x \in (R_+)^3 \mid 3k_3 > 0 \} \) with \( Y_{I_F}I_K \Psi(x) = 0 \) deforms by Theorem 4.18. Since \( I_F = I_\tilde{F} \), we can immediately discuss the case for fixed $k_3$ and solve simpler equations associated to the simplices of the triangulation. In case (1), for the cell with indices $(1, 2, 3, 5)$, the simpler equations are with $z = j_1 E_1 + j_4 E_4 = (j_1 + j_4, j_1, j_4, 0, j_4, 0)$

\[
\frac{z_2}{z_1} = \frac{j_1}{j_1 + j_4} = \tilde{k}_1^C w_1, \quad \frac{z_5}{z_3} = 1 = \tilde{k}_2^C w_2, \quad \frac{z_3}{z_1} = \frac{j_4}{j_1 + j_4} = \tilde{k}_3^C w_3
\]

yielding

\[
x = (w_1, w_3, w_1 w_2 w_3) = \left( \frac{j_1}{(j_1 + j_4)k_1^C}, \frac{j_4}{(j_1 + j_4)k_3}, \frac{j_1 j_4}{(j_1 + j_4)^2 k_1^C k_2^C k_3} \right).
\]

For $j_1 = 0, j_4 = 1$ the curve is touching a space \( \{ x \mid x_2 + x_3 = c_1 \} \) which is also true in a neighborhood, see Fig. 9. For the second cell $(1, 3, 5, 6)$ and $z = j_3 E_3 + j_4 E_4 = (j_4, 0, j_4, 0, j_3 + j_4, j_3)$ we solve

\[
\frac{z_5}{z_3} = \frac{j_3 + j_4}{j_4} = \tilde{k}_2^C w_2, \quad \frac{z_6}{z_3} = \frac{j_3}{j_4} = \frac{1}{\tilde{k}_1^C w_1}, \quad \frac{z_3}{z_1} = 1 = \tilde{k}_3 w_3,
\]

yielding

\[
x = \left( \frac{j_4}{j_3 k_1^C}, \frac{1}{k_3}, \frac{(j_3 + j_4)}{j_3 k_1^C k_2^C k_3} \right).
\]
When \( j_1 \) is small \( x \) is dominated by \( j_4 \) for both cells. The dependence is given by \( \mu = (1, 0, 1) \), the normal on the joint face. This agrees with Bernstein’s second theorem.

For the first cell \((1, 2, 4, 6)\) in case \(2\) we have for \( z = j_1E_1 + j_5E_5 = (j_1, j_1 + j_5, 0, j_5, 0, j_5) \)

\[
\frac{z_2}{z_1} = \frac{j_1 + j_5}{j_1} = \tilde{k}_1^C w_1,
\frac{z_6}{z_4} = 1 = \frac{1}{k_1^C k_2^C} \frac{1}{w_1 w_2},
\frac{z_4}{z_1} = \frac{j_5}{j_1} = \tilde{k}_2^C \tilde{k}_3 w_2 w_3
\]

giving \( w_1 = \frac{j_1 + j_5}{j_1 k_1}, \quad w_2 = \frac{j_1}{(j_1 + j_5) k_2^C}, \quad w_3 = \frac{j_5(j_1 + j_5)}{j_1 k_3}, \) and yielding altogether

\[
x = \left( \frac{j_1 + j_5}{j_1 k_1}, \frac{j_5(j_1 + j_5)}{j_1 k_3} \right) = \left( \frac{j_1 + j_5}{j_1 k_1}, \frac{j_5(j_1 + j_5)}{j_1 k_3} \right).
\]

For cell \((2, 3, 4, 6)\) we have with \( z = j_2E_2 + j_5E_5 = (0, j_5, j_2, j_2 + j_5, 0, j_5) \)

\[
\frac{z_4}{z_3} = \frac{j_1 + j_5}{j_2} = \tilde{k}_3 w_2 w_3,
\frac{z_6}{z_3} = \frac{j_5}{j_2} = \frac{1}{k_1^C w_1},
\frac{z_3}{z_2} = \frac{j_2}{j_5} = \tilde{k}_3 w_3
\]

yielding

\[
x = \left( \frac{j_2}{j_5 k_1^C}, \frac{j_2^2(j_2 + j_5)}{j_5 k_3}, \frac{j_2(j_2 + j_5)}{k_1^C k_2^C k_3} \right),
\]

For both cells, for small values of \( j_1, j_2 \) the solutions depend on \( j_5 \) like \( \mu = (1, 2, 2) \), the normal to the inner face of the regular triangulation. This agrees with Bernstein’s second theorem.

Figure 9 shows the real curves for \( k_0 = \tilde{k}_1 = \tilde{k}_2 = \tilde{k}_3 = 1 \) fixed and for two pairs of values of \( k_{g4}, \tilde{k}_{435}, \) e.g., \( k_{g4} = \tilde{k}_{435} = 0.1 \) and \( k_{g4} = \tilde{k}_{435} = 5 \).
Example 3.11 (continued). The lattice associated to the Cayley-graph-polytope is generated by \( y_2 - y_1, y_4 - y_3, y_6 - y_5 \) and has dimension 2. The lattice generated by \( y_2 - y_1, y_3 - y_1, y_4 - y_1, y_5 - y_1 \) has dimension 3. According to this, we choose the change of coordinates

\[
\begin{align*}
x_1 &= \frac{w_1}{w_2}, & x_2 &= \frac{w_1}{w_2 w_3}, & x_3 &= \frac{w_1}{w_2 w_3}, \\
& & & \text{and} & w_1 &= \frac{x_2}{x_1}, & w_2 &= \frac{x_3}{x_2}, & w_3 &= \frac{x_4}{x_1}.
\end{align*}
\]

For the change of coordinates on the rate constants we introduce a dummy parameter \( k_{6,6} \) since \( C_6 \) is a pure product complex. According to the lattices and the confluent vector \( g_3 = I_0 E_3 = I_0 (0, 1, 0, 0, 0) = (1, -1, 1, -1, -1, 1) \) we choose

\[
\begin{align*}
k_0 &= \frac{k_2^4}{k_1}, & k_1 &= \frac{k_1 k_2}{k_2}, & k_2 &= \frac{k_3^4}{k_4}, & k_3 &= \frac{k_4^3}{k_2}, \\
k_g &= \frac{k_2 k_4 k_6}{k_1}, & \hat{k} &= \frac{k_2^4 k_6}{k_1}, & k_{2,1} &= \frac{k_2 k_4 k_6}{k_1}, & k_{1,2} &= \frac{k_2 k_4 k_6}{k_3}, & k_{4,3} &= \frac{k_2 k_4 k_6}{k_3}, & k_{4,3} &= \frac{k_2 k_4 k_6}{k_3}, \\
k_{3,4} &= \frac{k_2 k_4 k_6}{k_3}, & k_{6,5} &= \frac{k_2 k_4 k_6}{k_3}, & k_{6,6} &= \frac{k_2 k_4 k_6}{k_3}.
\end{align*}
\]

In these coordinates a Gröbner basis of \( I_{g_3}^{\text{def}} \) with respect to a weighted order is

\[
\begin{align*}
z_4 z_6 &= k_g \hat{k} z_2^2, & \hat{k} z_1 z_2 z_3 &= z_2^2 z_5, & z_1 z_2 z_6 &= k_g z_2 z_4 z_5.
\end{align*}
\]

The ideal includes \( I_{g_3}^{\text{def}} = (z_1 z_3 z_6 - k_g z_2 z_4 z_5) \) and \( I_{g_3}^{\text{def}} = (z_4^2 z_5 - \hat{k} z_1 z_2 z_3) \).

The limit \( 1/k_g \to 0 \) deforms \( I_{g_3}^{\text{def}} \) to a monomial ideal with primary decomposition \((z_2) \cap (z_4) \cap (z_5)\). This corresponds to a regular triangulation of the Cayley-graph-polytope with three tetrahedra. The intersection of \( V(\langle z_2 \rangle) \) with \( (z_4) \) is a pure product complex. The subsystems have only complex balancing solutions. There is no multistationarity in the limit.

The limit \( k_g \to 0 \) deforms \( I_{g_3}^{\text{def}} \) to the monomial ideal \((z_1 z_3 z_6)\). The triangulation of the Cayley-graph-polytope consists of three tetrahedra. The intersections of the varieties with the cone are \( \text{cone}(E_2, E_3, E_4) \), \( \text{cone}(E_1, E_3, E_4) \), \( \text{cone}(E_1, E_2, E_3) \). The set \( \{ x \in \mathbb{R}_+^4 \mid \exists \hat{k} > 0 \text{ with } Y L_I Y_g \Psi(x) = 0 \} \) deforms to three sets of solutions of the subsystems. Here, only \( w_1, w_2 \) are determined.
For fixed \( \hat{k} \) we need to study a deformation \( \text{I}_{\text{def}} \). Term orders are elements of \( \ker(\hat{Y}_e) \) which includes \( \ker(\tilde{Y}_e) \). In this example \( w = g_3 \) is already a term order and in \( g_3(\text{I}_{\text{def}}^{\text{def}}) = \langle z_4 z_6, z_1 z_4 z_3, z_1 z_3 z_6 \rangle \) with primary decomposition

\[
\langle z_1, z_4 \rangle \cap \langle z_1, z_6 \rangle \cap \langle z_3, z_4 \rangle \cap \langle z_3, z_6 \rangle \cap \langle z_2, z_6 \rangle.
\]

Associated to this there is a regular triangulation of \( \text{conv}(y_1, y_1, y_3, y_4, y_5, y_6) \) with five tetrahedra, see Fig. 10. The intersections of the five protective spaces with the cone are \( \text{cone}(E_4) \), \( \text{cone}(E_2, E_3) \), \( \text{cone}(E_1, E_4) \), \( \text{cone}(E_1, E_3) \), \( \text{cone}(E_2) \). The second and fourth cell are interesting and the positive solutions of its subsystems are plotted in Fig. 10, together with the solution curve of the full system and the solutions of the subsystem associated to \( E_3 (14) \). The plot is for \( \hat{k}_1^C = \hat{k}_2^C = \hat{k}_3 = 1, \hat{k} = 10 $. Whether multistationarity arises still depends on the choice of \( B \).

The inner face (see Fig. 10) gives rise to multistationarity. Being an inner facet implies the inequalities \( \mu^t y_2 > \mu^t y_3, \mu^t y_4 < \mu^t y_5 \) which are part of the system of equalities and inequalities in [16].

Theorem 4.18 shows that the simplices of a regular triangulation of the Cayley-graph-polytope are the source of multistationarity. When the stoichiometric generators define inner faces of the regular triangulation, they can be considered as source of multistationarity as suggested by an example in [10]. The subsystem associated to an inner face given by a stoichiometric generator has positive solutions and thus guarantees that two neighboring simplices have positive solutions. But we need to restrict to those stoichiometric generators whose support involve several connected components. This theorem enables also an explanation of Femberg’s work on multistationarity [16].
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