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A Family of Sparse Polynomial Systems Arising in Chemical Reaction Systems

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The positive steady states of chemical reaction systems modeled by mass action kinetics are investigated. This sparse polynomial system is given by a weighted directed graph and a weighted bipartite graph. In this application the number of real positive solutions within certain affine subspaces of $\mathbf{R}^m$ is of particular interest. We show that the simplest cases are equivalent to binomial systems and are explained with the help of toric varieties. The argumentation is constructive and suggests algorithms. In general the solution structure is highly determined by the properties of the two graphs. We explain how the graphs determine the Newton polytopes of the system of sparse polynomials and thus determine the solution structure. Results on positive solutions from real algebraic geometry are applied to this particular situation. Examples illustrate the theoretical results.

1. Introduction

We investigate a class of sparse polynomial systems which come from applications. These systems arise in the modeling of chemical reaction systems by the so-called *mass action kinetics*. The polynomials in the system are defined by two graphs, a weighted directed graph for the chemical reactions and a weighted bipartite graph for the involved chemicals. An introduction to graph theory may be found in Diestel (1997).

In the non-algebraic chemical literature (Horn and Jackson, 1972; Feinberg and Horn, 1977; Clarke, 1980; Feinberg, 1979, 1987, 1988, 1991; Schlosser and Feinberg, 1994) there have been several attempts to study the number of real positive solutions depending on the structure of the graphs while dynamic phenomena have been greatly studied by numerical mathematicians (see, for example, Ebert *et al.*, 1981).

The investigation of real positive solutions of the sparse polynomial system $f(x) = 0$ is very important for the application since these are the steady state solutions of a dynamical system $\dot{x} = f(x)$. As a second motivation we mention singular perturbation theory. This theory exploits the knowledge of the real variety of $f(x) = 0$ for the investigation of properties of periodic orbits of $\dot{x} = f(x)$. A decomposition into slow and fast variables is done in cases where a periodic orbit is close to the real variety. For another motivation observe that $f(x)$ may be the reaction part of a partial differential equation of reaction-diffusion type. The dependence of the steady states on the parameter (e.g. a coefficient

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of a monomial) influences the existence of time- and space-dependent solutions of the reaction diffusion system.

The study of positive solutions by chemists and applied mathematicians is completely independent of the literature on sparse polynomial systems in algebraic geometry. There are at least four methods for dealing with sparse polynomial systems: Gröbner bases, characteristic sets, sparse resultants, and homotopy methods. In Melenk *et al.* (1989) Gröbner basis computations for systems of mass action type have been performed. We do not follow this approach. The homotopy method (Huber and Sturmfels, 1995) is a mixed discrete-numeric algorithm in order to find all complex solutions of the sparse polynomial system. It is based on subdivisions of the Newton polytopes associated to the sparse equations. Based on this a wide range of articles appeared (see, for example, Verschelde and Gatermann 1995; Verschelde *et al.* 1996; Huber and Verschelde 1998; Gao *et al.* 1999).

Related to this approach there are results on the number of real and positive real solutions (Itenberg and Roy, 1996; Sturmfels, 1994a,b). In Sturmfels (1998) an easy to read summary of these approaches is presented. In the last section we apply this method to our particular situation.

The aim of this paper is to build a bridge between the two areas, the applied mathematics literature and the algebraic literature on sparse polynomial systems. We give a mathematical introduction into the model and algebraic proofs of the results in the non-algebraic literature. The application of the results of sparse polynomial systems gives a deeper understanding and transparency and leads to new algorithms. Since the problem is formulated by graphs all results have a graph theoretic interpretation. Our main result is that the Newton polytopes show that parts of the directed graph are closely related to the existence of positive solutions for various choices of rate constants.

The outline of the paper is as follows. In Section 2 we give a detailed description of the problem, the sparse polynomial system $YA\Psi(x) = 0$. Since the coefficients are heavily determined by the structure of the matrix A this structure is investigated in Section 3. Section 4 gives the general structure of the equations. Sections 5–7 deal with special simple cases without mixed equations. Some systems do not have positive solutions. Some systems can be decoupled explicitly. Other systems are equivalent to binomial systems. Systems satisfying the assumptions of the Deficiency One Theorem have precisely one positive solution. The mathematical tools are Smith normal form and Hermite normal form from linear algebra and toric varieties from algebraic geometry.

Finally, the last section applies the theory of sparse polynomial systems using mixed subdivisions of Newton polytopes.

Examples illustrating the theoretical results have been computed with the help of Maple.

2. The Model of Mass Action Kinetics

Chemical reactions are determined by the reacting chemicals and some rules for possible reactions which transfer one group of chemicals into another group of chemicals.

A mathematical description of this information is given by two graphs. First there is a *weighted directed graph* R with *oriented edges* $C_j \to C_i$ for some $i, j \in \{1, \ldots, n\}$ linking the vertices C_i. Each oriented edge (arrow) $C_j \to C_i$ has a weight $k_{C_j \to C_i} = k_{ij} \in \mathbf{R}_+$. This information is encoded in the weighted adjacency matrix $K = (k_{ij}) \in (\mathbf{R}_{\geq 0})^{n,n}$ with $k_{ij} = 0$ if and only if $C_j \to C_i$ is not an arrow. The second graph is a *weighted bipartite*

graph encoding the occurrence of chemical *species* S_i in C_j. The two sets of vertices consist of the species S_i, $i = 1, \ldots, m$ and the C_j, $j = 1, \ldots, n$. Each edge $\{C_j\, S_i\}$ has a weight $y_{ij} \in \mathbf{N}$ and $y_{ij} = 0$ if and only if C_j and S_i are not adjacent. This defines the weighted adjacency matrix whose relevant part is $Y = (y_{ij})_{i=1,\ldots,m,j=1,\ldots,n}$. We denote the columns of Y by $y_1, \ldots, y_n \in (\mathbf{Z}_{\geq 0})^m$ and assume that they are all different.

REMARK. In the chemical literature the vertices C_i are called *complexes* while the weights k_{ij} of the edges are called *rate constants*. Y is called the *stoichiometric matrix* since the complexes are given as $C_j = \sum_{i=1}^{m} y_{ij} S_i$, $j = 1, \ldots, n$ with the so-called *stoichiometric coefficients* y_{ij}.

There are some non-degeneracy restrictions on the directed graph. For example, each C_i appears at least once in an oriented edge. A *forward reaction* $C_j \to C_i$ and an *anti-reaction* $C_i \to C_j$ with two different associated constants are simultaneously possible. But there are no parallel edges. Also some C_j may appear as results only, while others appear on the left of a reaction $C_i \to C_j$. The number of the latter is denoted by r. Obviously, $r \leq n$. In the bipartite graph it may happen that one C_j is not linked to any S_i and thus the associated column is $y_j = 0$. But we assume that every vertex S_i is adjacent to at least one vertex C_j.

REMARK. C_j which only appear as results are called *product complexes*. C_j appearing on the left of a reaction are called *reactant complexes*. A reaction $C_j \to C_\nu$ with a complex C_j not linked to any species S_i corresponds to the fact that the chemical species in C_ν are constantly poured into the chemical reactor.

In a stirred chemical reactor the behavior of the concentrations x_i of species S_i under chemical reaction is modeled by a system of autonomous ordinary differential equations. The model of *mass action kinetics* is built from three mappings resulting in a system given by sparse polynomials.

(1) The directed graph defines a linear mapping A which encodes the information about the reaction probabilities. The amount of reaction $C_j \to C_i$ taking place depends on the presence of the species in C_j in the reactor. The presence is measured by the quantity u_j. Then the chance that the reaction $C_j \to C_i$ actually happens is $k_{ij}u_j$ where k_{ij} is the associated positive constant. The reaction will decrease the amount of all species in C_j and increase the species in C_i. Let the unit vectors of $\mathbf{R}^n$ be denoted by $\omega_1, \ldots, \omega_n$. Then

$$A : \mathbf{R}^n \to \mathbf{R}^n, \qquad u \mapsto \sum_{(C_j \to C_i) \in R} k_{ij} u_j (\omega_i - \omega_j),$$

is a linear mapping measuring the changes. Since

$$Au = \sum_{(C_j \to C_i) \in R} k_{ij}\, u_j\, \omega_i - \sum_{(C_i \to C_j) \in R} k_{ji}\, u_i\, \omega_i = Ku - \sum_{i=1}^{n} \left(\sum_{j=1}^{n} k_{ji} \right) u_i\, \omega_i,$$

the matrix of the mapping A with respect to the standard basis $\omega_1, \ldots, \omega_n$ of $\mathbf{R}^n$ is the matrix $A = (K - \operatorname{diag}(K^t e))$, where $e = (1, \ldots, 1)^t \in \mathbf{R}^n$. An alternative presentation of A uses two *incidence matrices*. The first incidence matrix of the directed graph is $I_a = (w_{ij})_{i=1,\ldots,n,j=1,\ldots,a}$ where $w_{ij} \in \{-1, 0, 1\}$ and a denotes the number of arrows. Each column represents an oriented edge $C_j \to C_i$ by containing one entry -1 for C_j

and 1 for C_i. The second incidence matrix is $I_K = (\kappa_{\mu\nu})_{\mu=1,\dots,a,\nu=1,\dots,n}$ with $\kappa_{\mu\nu} \in \{k_{ij} \,|\, i,j = 1,\dots,n\}$ or $\kappa_{\mu\nu} = 0$. Each row corresponds to one oriented edge and has at most one non-zero entry. The μth arrow $C_j \to C_i$ gives $\kappa_{\mu j} = k_{ij}$ encoding the weight and that C_j is the reactant complex. With these notations

$$A = K - \operatorname{diag}(K^t e) = I_a \, I_K .$$

REMARK. In the chemical literature A is called the *kinetic matrix*.

Observe that $n - r$ columns of A corresponding to product complexes are zero.

(2) For each vertex C_j there is a monomial $x^{y_j} = \prod_{i=1}^m x_i^{y_{ij}}$ in the variables $x_1, \dots, x_m$ which are the concentrations of the species. Whenever something depends on the chance that the chemicals in C_j meet in the chemical reactor, the monomial x^{y_j} is involved. Thus we define

$$\Psi : \mathbf{R}^m \to \mathbf{R}^n, \qquad \Psi(x) = \begin{pmatrix} x^{y_1} \\ \vdots \\ x^{y_n} \end{pmatrix}.$$

The exponents y_j are the columns of the matrix Y while $y_{ij} = (y_j)_i$ denote the elements of $Y = (y_{ij})$. Often we will restrict Ψ to the non-negative orthant $(\mathbf{R}_{\geq 0})^n$ or to the positive orthant $(\mathbf{R}_+)^n$.

(3) The third mapping is the linear mapping

$$Y : \mathbf{R}^n \to \mathbf{R}^m, \qquad z \to \sum_{j=1}^n y_j z_j,$$

associated to the relevant part $Y = (y_1, \dots, y_n) \in (\mathbf{Z}_{\geq 0})^{m,n}$ of the weighted adjacency matrix of the bipartite graph. y_j is the j-column of Y while $y_{ij} = (y_j)_i$ denote the elements of $Y = (y_{ij})$. The change of the jth complex is $z_j = (Au)_j$. The chemical substance S_i appears in some of these C_j with coefficient y_{ij}. Thus $(Yz)_i$ gives the change of species S_i according to the changes of the complexes. The composition is

$$\begin{aligned} YA\,u = Y(K - \operatorname{diag}(K^t e))u &= \sum_{i=1}^n \sum_{j=1}^n y_i k_{ij} u_j - \sum_{j=1}^n y_j \sum_{i=1}^n k_{ij} u_j \\ &= \sum_{(C_j \to C_i) \in R} k_{ij} u_j (y_i - y_j). \end{aligned}$$

Altogether the chemical reaction is modeled by the differential equations

$$\dot{x} = YA\Psi(x). \tag{1}$$

An obvious property is that the monomials corresponding to pure product complexes do not appear in (1) because of the structure of A.

REMARK. Equation (1) is presented in this form by Feinberg. It is a special case of the systems investigated in Clarke (1980), Eiswirth (1994), Eiswirth *et al.* (1996), Gatermann (2000) and Heinrich and Schuster (1996, 1998) and references therein. Clarke uses the matrix $\underline{\nu} := YI_a$ which has the property that each column contains the stoichiometric

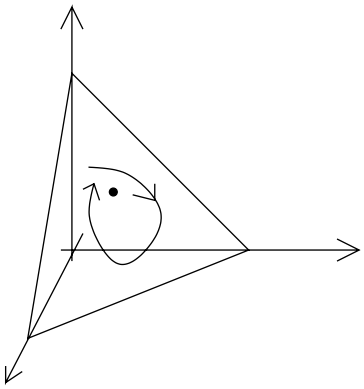

Figure 1. A trajectory within an affine subspace as in Lemma 2.1.

coefficients of the reactant complex *and* the product complex of one reaction, but with opposite sign. With $v(x) = I_K \Psi(x)$ system (1) is written as

$$\dot{x} = \underline{\nu}\, v(x). \tag{2}$$

In the general case the exponents of monomials in $\Psi(x)$ are *less* than or equal to y_{ij}. In the chemical literature the two graphs are represented as a diagram.

Remark. (i) It should be understood that the weighted directed graph and the weighted bipartite graph are often a description of the model after the actual problem has been simplified. Several oriented edges are often summarized as one edge by experience and by insight into the chemical process by chemical engineers. In the elementary reactions the complexes consist, most of the time, of two species only. (ii) A special case occurs if the chemical reaction only happens on the surface of a catalyst. Then the graphs have a more special structure. (iii) Often the model of mass action kinetics is modified by taking, instead of monomials, more general functions into account. (iv) The edge $0 \to S_i$ models pouring liquid into the reactor and $S_j \to 0$ taking some substance out: a steady state of the equations corresponds to a constant flow of the actual system.

When studying the differential equation (1) one is first interested in the steady state solutions in $(\mathbf{R}_+)^m$ or $(\mathbf{R}_{\geq 0})^m$ in its dependency of the graph structure.

Due to the structure arising from chemical reactions the systems will often be underdetermined. Thus one adds additional linear restrictions in order to find finitely many solutions. A natural choice are the affine linear subspaces $x_0 + \operatorname{im}(YA)$ since they are flow-invariant by the following lemma.

Lemma 2.1. *Let $\dot{x} = B\chi(x)$ be a differential equation with a vector of monomials $\chi(x) = (c_1 x^{d_1}, \ldots, c_l x^{d_l})^t$ with $c_i \in \mathbf{R} \setminus \{0\}, d_i \in (\mathbf{Z}_{\geq 0})^m, i = 1, \ldots, l$ and a matrix $B \in \mathbf{R}^{m,l}$. A solution trajectory $x : \mathbf{R} \to \mathbf{R}^m$ for the initial condition $x(t_0) = x_0 \in (\mathbf{R})^m$ stays for all $t > t_0$ within the affine space $x_0 + \operatorname{im}(B)$. Assume, additionally, that the constants c_i in χ are positive. If $x(t_0) = x_0 \in (\mathbf{R}_{\geq 0})^m$ then $x(t)$ stays for all $t > t_0$ in the* convex polyhedral cone $x_0 + \left\{ \sum_{j=1}^{l} \alpha_j B\omega_j \,|\, \alpha_j \geq 0, j = 1, \ldots, l \right\}$.

PROOF. The first statement is equivalent to the fact that for any $t_1 < t_2$ the vector $x(t_1) - x(t_2)$ is an element of $\mathrm{im}(B)$. Simple integration along the solution $x(t)$ yields

$$x(t_2) = x(t_1) + \int_{t_1}^{t_2} B\chi(x(t))\,dt.$$

This is equivalent to

$$x(t_2) - x(t_1) = B\int_{t_1}^{t_2} \chi(x(t))\,dt,$$

which shows that the difference $x(t_2) - x(t_1)$ is a linear combination of the columns of B with coefficients $\alpha_j = \int_{t_1}^{t_2} \chi_j(x(t))\,dt = \int_{t_1}^{t_2} c_j x(t)^{d_j}\,dt$.

If $x(t)$ is non-negative then the monomial vector χ is non-negative by the positiveness of the constants c_i and so are the coefficients α_j. □

A trajectory in the positive orthant $(\mathbf{R}_{\geq 0})^m$ staying in the cone $x_0 + \sum_j \alpha_j B\omega_j$ stays in particular in $(x_0 + \mathrm{im}(B)) \cap (\mathbf{R}_{\geq 0})^m$. In our context two special cases of B are interesting.

COROLLARY 2.2. *For the differential equation $\dot{x} = YA\Psi(x)$ each affine space $x_0 + \mathrm{im}(YA)$ is flow-invariant. In particular $((x_0 + \mathrm{im}(YA)) \cap (\mathbf{R}_{\geq 0})^m$ for any $x_0 \in \mathbf{R}^m$ is flow-invariant.*

PROOF. Apply Lemma 2.1 with $B = YA$ and $\chi = \Psi$. □

COROLLARY 2.3. *For the differential equation $\dot{x} = YI_aI_K\Psi(x)$ each affine space $x_0 + \mathrm{im}(YI_a)$ is flow-invariant. In particular $((x_0 + \mathrm{im}(YI_a)) \cap (\mathbf{R}_{\geq 0})^m$ for any $x_0 \in \mathbf{R}^m$ is flow-invariant.*

PROOF. Apply Lemma 2.1 with $B = YI_a$ and $\chi = I_K\Psi = v$. □

REMARK. In Feinberg (1987) the vector space $\mathrm{im}(YA)$ is called *kinetic space* and $S = \mathrm{im}(YI_a) = \mathrm{span}(\{y_i - y_j \,|\, (C_j \to C_i) \in R\})$ is called *stoichiometric space*. Obviously, $\mathrm{im}(YA) \subseteq S$. In Section 3 we will give a sufficient condition for $\mathrm{im}(YA) = S$. Choosing different sets of constants $\{k_{ij} \,|\, (C_j - C_i) \in R\}$ in general the linear space $\mathrm{im}(YA)$ will vary with the choices of k_{ij} since the matrix A depends on these constants. However, for many problems arising in applications we have $\mathrm{im}(YA) = S$.

Let $v_i, i = 1, \ldots, m - \mathrm{rank}(YA)$ denote an orthonormal basis of the orthogonal complement of $\mathrm{im}(YA)$. That means the v_i form a basis of $\ker((YA)^t)$. As known from elementary linear algebra the condition $x \in (x_0 + \mathrm{im}(YA))$ is equivalent to $v_i^t x - a_i = 0$, $i = 1, \ldots, m - \mathrm{rank}(YA)$, for $a_i = v_i^t x_0 \in \mathbf{R}$.

One would like to choose all v_i to be non-negative, but in general the dimension of the convex polyhedral cone $\ker((YA)^t) \cap (\mathbf{R}_{\geq 0})^m$ may be smaller than $\dim(\ker(YA)^t)$ (for an example, see Heinrich and Schuster, 1996).

REMARK. If a vector v_i is non-negative then $v_i^t x - a_i = 0$ is called the *conservation relation* and v_i is called the *conservation vector* since the physical meaning is that a quantity is conserved.

We formulate the problem more precisely:

PROBLEM 2.4. Given a weighted directed graph with adjacency matrix $K = (k_{ij}) \in (\mathbf{R}_{\geq 0})^{n,n}$ and incidence matrices I_a, I_K and matrix $A = I_a I_K$. Given a weighted bipartite graph with matrix $Y = (y_1, \ldots, y_n) = (y_{ij}) \in (\mathbf{Z}_{\geq 0})^{m,n}$. We choose a basis $\{v_i\}$ of $\ker((YA)^t)$ and constants $a_i \in \mathbf{R}$. We are interested in the solutions in $(\mathbf{R}_{\geq 0})^m$ or $(\mathbf{R}_+)^m$ of

$$YA\Psi(x) = 0, \qquad v_i^t x - a_i = 0, \qquad i = 1, \ldots, m - s, \tag{3}$$

$s = \operatorname{rank}(YA)$ depending on the choices of the constants a_i and the rate constants k_{ij}. Especially, it is interesting to know whether the number of solutions depends on the choices of a_i when the constants k_{ij} are fixed.

We will investigate Problem 2.4 in the context of algebraic geometry where a system of sparse Laurent polynomials in the variables $x_1, \ldots, x_m$ is written as

$$f^{ij}(x) = \sum_{a \in \mathcal{A}_i} c_a^{ij}\, x^a = 0, \qquad j = 1, \ldots, k_i, \qquad i = 1, \ldots, r, \tag{4}$$

where $k_1 + \cdots + k_r = m$ and $c_a^{ij} \in \mathbf{C}$ are constants and the supports $\mathcal{A}_i \subset \mathbf{Z}^m$ have finite order. The most important objects are the *Newton polytopes* and the *lattice*. For an introduction to the general theory of polytopes see Ziegler (1995).

DEFINITION. The *Newton polytope* of a sparse polynomial $f^{ij}(x)$ with support $\mathcal{A}_i \subset \mathbf{Z}^m$ is the convex hull of the points $a \in \mathcal{A}_i$. This polytope in $\mathbf{R}^m$ is denoted by $\operatorname{conv}(\{a \,|\, a \in \mathcal{A}_i\})$. The *lattice* of one sparse polynomial $f^{ij}(x)$ with support $\mathcal{A}_i \subset \mathbf{Z}^m$ is the $\mathbf{Z}$-module generated by all $a - b$, $b \in \mathcal{A}_i \setminus \{a\}$, where one element $a \in \mathcal{A}_i$ is chosen fixed. The *lattice* of the *system* of sparse polynomials $f^{ij}(x)$ with supports $\mathcal{A}_i \subset \mathbf{Z}^m$, $i = 1, \ldots, r$ is the sum of the lattices of the single polynomials.

The naive way of looking at equation (3) is to identify $(YA\Psi)_k, k = 1, \ldots, m$ and $v_i^t x - a_i$ as sparse polynomials. But YA does not have full rank and one would like to perform linear algebra operations first. Before using the results from algebraic geometry one uses linear algebra in order to find supports as sparse as possible. On the other hand the coefficient matrix YA depends on the structure of the graphs. That is why the literature (Feinberg and Horn, 1977) starts with the investigation of the kinetic matrix A.

3. The Structure of the Matrix $A = I_a I_K$

Since the matrix A depends on the structure of the directed graph the basic properties of a directed graph are recalled first.

Ignoring the orientation of the edges we have a multi-graph. A standard notion of a graph is that of its *connected components*. We refer to them as $\mathcal{L}_\lambda \subset \{1, \ldots, n\}$, $\lambda = 1, \ldots, l$ collecting the indices of connected vertices. Thus $\{1, \ldots, n\} = \mathcal{L}_1 \dot\cup \mathcal{L}_2 \dot\cup \cdots \dot\cup \mathcal{L}_l$. Analogously, we decompose the set of indices of oriented edges $\{1, \ldots, a\}$ into $\mathcal{E}_\lambda$ corresponding to connected components.

Since the graph is directed the connected components may be even further decomposed. While a cycle $C_i \to C_{j_1} \to C_{j_2} \leftarrow C_{j_3} \to \cdots \leftarrow C_{j_k} \to C_i$ (arrows in one or the other direction) is called a *circuit* in matroid theory (Björner *et al.*, 1993) a cycle with

all arrows in the same direction is called a *positive circuit*. Two vertices C_i, C_j on a positive circuit are called *strongly linked* (Feinberg, 1979, pp. 4–7). A maximal set of vertices which are pairwise strongly linked is called the *strong connected component*. If no C_j in a strong connected component reacts to a C_i not in this component, this component is called the *terminal strong connected component*. We denote these terminal components by $\mathcal{T}_\lambda^\nu \subset \{1,\dots,n\}, \nu = 1,\dots,t_\lambda$ where $t_1 + \cdots + t_l = t$ is their total number. Accordingly, the set of arrows decompose into $\mathcal{E}_\lambda^\nu \subset \{1,\dots,a\}, \nu = 1,\dots,t_\lambda$ for the terminal strong connected components. For the arrows *between* strong connected components we introduce the index set $\mathcal{C}_\lambda \subseteq \mathcal{E}_\lambda \setminus \bigcup_\nu \mathcal{E}_\lambda^\nu$.

LEMMA 3.1. *The vector space* $\mathbf{C}^n$ *decomposes into vector spaces according to the connected components which are invariant under* A*, i.e.* $L_\lambda = \operatorname{span}(\{\omega_i \,|\, i \in \mathcal{L}_\lambda\})$ *with*

$$\mathbf{C}^n = L_1 \oplus \cdots \oplus L_l \qquad \text{and} \qquad AL_\lambda \subset L_\lambda, \qquad \lambda = 1,\dots,l.$$

Each L_λ *further decomposes according to the terminal strong connected components, i.e. for each* $\lambda = 1,\dots,l$ *one defines* $T_\lambda^\nu = \operatorname{span}(\{\omega_i \,|\, i \in \mathcal{T}_\lambda^\nu\})$ *for* $\nu = 1,\dots,t_\lambda,\ \lambda = 1,\dots,l$ *and the rest* $R_\lambda = \operatorname{span}\left(\left\{\omega_i \,|\, i \in \mathcal{L}_\lambda \setminus \bigcup_{\nu=1}^{t_\lambda} \mathcal{T}_\lambda^\nu\right\}\right)$*. Then for all* $\lambda = 1,\dots,l$

$$L_\lambda = T_\lambda^1 \oplus \cdots \oplus T_\lambda^{t_\lambda} \oplus R_\lambda \qquad \text{with} \quad AT_\lambda^\nu \subset T_\lambda^\nu, \qquad \nu = 1,\dots,t_\lambda.$$

PROOF. The matrix A decomposes according to the connected components and terminal strong connected components after a permutation of rows and columns as

$$A = \begin{pmatrix} A_1 & & \\ & \ddots & \\ & & A_l \end{pmatrix}, \qquad A_\lambda = \begin{pmatrix} B_0 & 0 & \cdots & 0 \\ B_1 & A_{\lambda 1} & & 0 \\ \vdots & & \ddots & \\ B_{t_\lambda} & 0 & & A_{\lambda t_\lambda} \end{pmatrix}, \qquad \lambda = 1,\dots,l.$$

The connected components give a block structure of I_a and I_K with blocks $((I_a)_{ij})_{i\in\mathcal{L}_\lambda, j\in\mathcal{E}_\lambda}$ and $((I_K)_{ij})_{i\in\mathcal{E}_\lambda, j\in\mathcal{L}_\lambda}$. All entries outside these blocks are zero. Then $A_\lambda = ((A)_{ij})_{i,j\in\mathcal{L}_\lambda}$ is the product of blocks, which means that L_λ is invariant.

Analogously, the blocks $A_{\lambda\nu}$ associated to terminal strong connected components are the product of blocks $((I_a)_{ij})_{i\in\mathcal{L}_\lambda^\nu, j\in\mathcal{E}_\lambda^\nu}$ and $((I_K)_{ij})_{i\in\mathcal{E}_\lambda^\nu, j\in\mathcal{L}_\lambda^\nu}$. This gives the invariant space $\mathcal{T}_\lambda^\nu$. The remaining block $B = ((A)_{ij})_{i\in\mathcal{L}_\lambda, j\in\mathcal{L}_\lambda\setminus\cup_\nu\mathcal{T}_\lambda^\nu}$ is the product of two sub-blocks $((I_a)_{ik})_{i\in\mathcal{L}_\lambda, k\in\mathcal{E}_\lambda\setminus\cup_\nu\mathcal{E}_\lambda^\nu}$ and $((I_K)_{kj})_{k\in\mathcal{E}_\lambda\setminus\cup_\nu\mathcal{E}_\lambda^\nu, j\in\mathcal{L}_\lambda\setminus\cup_\nu\mathcal{T}_\lambda^\nu}$ yielding $AR_\lambda \subset L_\lambda$. □

The next theorem states that each terminal strong connected component gives a kernel vector of A.

THEOREM 3.2. (FEINBERG AND HORN, 1977, PROPOSITION 4.1 IN FEINBERG, 1979) *We assume that the constants* k_{ij} *in the matrix* I_K *are positive if* $C_j \to C_i$ *is an edge in the directed graph and* $k_{ij} = 0$ *if and only if* $C_j \to C_i$ *is not an edge. The kernel of the matrix* $A = I_a I_K = K - \operatorname{diag}(K^t e)$ *decomposes as*

$$\ker(A) = \bigoplus_{\lambda=1}^{l} \bigoplus_{\nu=1}^{t_\lambda} (\ker(A) \cap T_\lambda^\nu).$$

Moreover, $\dim(\ker(A) \cap T_\lambda^\nu) = 1,\ \nu = 1,\dots,t_\lambda,\ \lambda = 1,\dots,l$ *and there exist generating vectors* $v_\lambda^\nu \in (\mathbf{R})^n$ *which are non-negative and have support* $\mathcal{T}_\lambda^\nu$*, that means*

$$(v_\lambda^\nu)_i > 0 \qquad \textit{for all } i \in \mathcal{T}_\lambda^\nu, \qquad (v_\lambda^\nu)_i = 0 \qquad \textit{for all } i \in \{1,\dots,n\} \setminus \mathcal{T}_\lambda^\nu.$$

In other words $\ker(A)$ *equals* $\operatorname{span}(\{v_\lambda^\nu \mid \lambda = 1,\dots,l, \nu = 1,\dots,t_\lambda\})$.

PROOF. By the block structure it is clear that $\ker(A) = \oplus_\lambda \ker(A) \cap L_\lambda$. Moreover, we may restrict ourselves to the case that there are no pure product complexes and thus I_K has maximal rank. Otherwise each pure product complex forms one terminal strong connected component. Thus each index i corresponding to a pure product complex gives a unit vector ω_i in the kernel of A and consequently an invariant space $T_\lambda^\nu = \operatorname{span}(\omega_i)$.

Since I_K has maximal rank we only need to investigate kernel vectors $w \in \ker(I_a)$ and then solve $w = I_K v$, if possible. But $\ker(I_a)$ is generated by vectors associated to circuits.

First we investigate terminal strong connected components and its associated blocks $A_{\lambda\nu}$ since they give invariant subspaces. The kernel of I_a restricted to this $(\ker(I_a) \cap \operatorname{span}(\{\omega_i \mid i \in \mathcal{E}_\lambda^\nu\}))$ is generated by positive circuits within this terminal strong connected component. Thus w is a linear combination of positive circuits. Since A has the representation $K - \operatorname{diag}(K^t e)$ the block $A_{\lambda\nu}$ also has such a representation. But $e^t(K - \operatorname{diag}(K^t e)) = e^t K - e^t K = 0$. This yields $\dim(\ker(A) \cap T_\lambda^\nu) \geq 1$. If the dimension was two or larger there would be a kernel vector v of $A_{\lambda\nu}$ with $v_i = 0$ for one $i \in \mathcal{T}_\lambda^\nu$. Then for each circuit $C_i \xrightarrow{e_1} C_{j_1} \xrightarrow{e_2} C_{j_2} \xrightarrow{e_3} \cdots \xrightarrow{e_k} C_{j_k} \xrightarrow{e_{k+1}} C_i$ we have $(I_K v)_{e_1} = 0$. Since the columns of $((I_a)_{k\kappa})_{k\in\{i,j_1,\dots,j_k\},\kappa\in\{e_2,\dots,e_{k+1}\}}$ are linearly independent $w_\kappa = (I_a v)_\kappa = 0, \kappa \in \{e_2,\dots,e_{k+1}\}$ and thus $v_{j_\mu} = 0, \mu = 1,\dots,k$ by the maximal rank of I_K. Since C_i is strongly linked to all $j \in \mathcal{T}_\lambda^\nu$ it follows $v = 0$ and thus $\dim(\ker(A) \cap \mathcal{T}_\lambda^\nu) = 1$.

Let $w \in \ker(I_a)$ be a linear combination of vectors corresponding to circuits within one non-terminal strong connected component. Then for v with $I_K v = w$ we have $v_i \neq 0$ for all i with C_i in this strong connected component by the argumentation earlier. But then $w_j \neq 0$ for some $j \in \mathcal{C}_\lambda$ (some arrow pointing out) contradicting the assumption.

For some graphs there exists no circuit involving arrows from $\mathcal{C}_\lambda$ connecting non-terminal and terminal strong connected components. Then the proof is complete.

So we assume in general that the linear combination of a kernel vector $w \in \ker(I_a)$ involves a circuit with arrows from $\mathcal{C}_\lambda$. Then there exists a non-terminal strong connected component and two arrows $C_i \xrightarrow{\mu} C_j$ and $C_\chi \xrightarrow{\kappa} C_\xi$ (pointing out) such that $w_\mu < 0$ and $w_\kappa > 0$. Because rate constants k_{ij} are positive $v_i < 0$ and $v_\chi > 0$. Looking at positive circuits within the non-terminal strong connected component involving C_i and C_χ we conclude as earlier that all v_μ for all C_μ in this component have the same sign. This gives a contradiction and no such kernel vectors $w \in \ker(I_a)$ exist. □

The theorem states that each block $A_{\lambda\nu}$ has rank defect one and each block A_λ has rank defect t_λ, the number of terminal strong connected components within the connected component λ. Thus $\operatorname{rank}(A) = n - t$ where t is the total number of terminal strong connected components.

The following defines a case with a simple structure of A.

DEFINITION. (FEINBERG, 1979) The directed graph is called *weakly reversible* if all its connected components are strong connected components.

In a weakly reversible graph each connected component equals its terminal strong connected component. For weakly reversible graphs we have $\operatorname{rank}(A) = n - l$ where l is

the number of connected components. But $\operatorname{rank}(A) = n - l$ may be true for graphs which are not weakly reversible. For the latter, it is sufficient that each connected component contains precisely one terminal strong connected component ($t_\lambda = 1$, $\lambda = 1, \ldots, l$).

4. The Structure of the Equations

In this paragraph we restrict ourselves, for simplicity, to directed graphs which are weakly reversible. By elementary linear algebra we transform the equations $YA\Psi(x) = 0$ into the form of system (4) with supports as sparse as possible.

For the coefficient matrix we use the decompositions $Y_\lambda = (y_{ij})_{i=1,\ldots,m, j\in\mathcal{L}_\lambda}$ and $A_\lambda = (a_{ij})_{i,j\in\mathcal{L}_\lambda}$. After we have performed some linear algebra operation on $YA\Psi(x)$ the number of polynomials involving monomials from the connected component λ only is

$$k_\lambda = \operatorname{rank}(YA) - \operatorname{rank}(Y_1A_1 \cdots \widehat{Y_\lambda A_\lambda} \cdots Y_lA_l)), \qquad \lambda = 1, \ldots, l,$$

where $\widehat{Y_\lambda A_\lambda}$ means to leave out this block. After linear algebra transformations there remain $k_{l+1} = \operatorname{rank}(YA) - \sum_{\lambda=1}^{l} k_\lambda$ polynomials (called *mixed*) involving monomials from more than one connected component. Finally, $k_{l+2} = m - \operatorname{rank}(YA)$ linear relations complete the set of equations.

$$\begin{aligned}
\sum_{j\in\mathcal{L}_\lambda} c_{ij}\, x^{y_j} &= 0, \qquad i = 1, \ldots, k_\lambda, \qquad \lambda = 1, \ldots, l,\\
\sum_{j=1}^{n} b_{ij}\, x^{y_j} &= 0, \qquad i = 1, \ldots, k_{l+1},\\
v_i^t\, x - a_i &= 0, \qquad i = 1, \ldots, k_{l+2}.
\end{aligned} \tag{5}$$

The coefficients c_{ij} and b_{ij} depend on the rate constants and the structure of the graphs.

Studying the solutions of $YA\Psi(x) = 0$ within affine shifts of $\operatorname{im}(YA)$ is equivalent to studying system (5).

Remark. (i) The number of mixed equations in the second group is usually small, just $1, 2$ or 3. The support is the collection of supports of the first polynomials. Sometimes one may even further distinguish the supports of the k_{l+1} mixed equations. (ii) The Newton polytopes are of a particular structure. For the linear relations they are simplices.

Since the linear algebra of the coefficient matrix $YA = YI_aI_K$ is so important, Feinberg (1979) calls $\delta = \operatorname{rank}(I_a) - \operatorname{rank}(YI_a) = n - l - \operatorname{rank}(YI_a) = n - l - \dim(S)$ the *deficiency* where l is the number of connected components. In case the directed graph is weakly reversible δ agrees with $\operatorname{rank}(A) - \operatorname{rank}(YA)$, but if one connected component has several terminal strong connected components than $\operatorname{rank}(A) < \operatorname{rank}(I_a)$ and $\operatorname{rank}(A) - \operatorname{rank}(YA) < \delta$ may be possible.

In the following sections we consider a simple case for a graph which is not weakly reversible and several results for weakly reversible graphs *without* mixed equations. Finally, we investigate the general case *with* mixed equations.

5. A Case Without Positive Solutions

In the following a system of mass action kinetics is investigated where the directed graph is not weakly reversible and an equation with a zero-dimensional Newton polytope

is included. Then the mixed volume of the Newton polytopes is zero. By Bernstein's theorem, the mixed volume of the Newton polytopes gives the number of complex solutions in $(\mathbf{C} \setminus \{0\})^m$ for generic coefficients, see Cox *et al.* (1998).

LEMMA 5.1. *Consider the system* $YA\Psi(x) = YI_aI_K\Psi(x) = 0$ *given by a weighted directed graph with adjacency matrix* K *and incidence matrices* I_a *and* I_K *and a weighted bipartite graph with matrix* Y*. Assume that the directed graph is not weakly reversible and there exists an index* $i \in \mathcal{R} = \bigcup_\lambda \left(\mathcal{L}_\lambda \setminus \bigcup_\nu \mathcal{T}_\lambda^\nu\right)$ *in the non-terminal part such that* Ya_i *is linearly independent of the other columns* $Ya_j, j \in \{1, \ldots, n\} \setminus \{i\}$*, where* a_i *denotes the* i*th column of* A*. If* $y_i \neq \mathbf{0}$ *then the system* $YA\Psi(x) = 0$ *has no solutions in* $(\mathbf{C} \setminus \{0\})^m$*. Especially, it has no positive real solutions. If* $y_i = \mathbf{0}$ *then* $YA\Psi(x) = 0$ *has no solution at all.*

PROOF. The assumptions are such that by linear algebra an equation $x^{y_i} = 0$ has to be satisfied. If $y_i \neq \mathbf{0}$ this can only be satisfied if some component $x_j = 0$ where j is in the support of y_i. The case $y_i = \mathbf{0}$ yields the unsolvable equation $1 = 0$. □

EXAMPLE 5.2. A model introduced by Heinmets (see also Bock, 1981 and Melenk *et al.*, 1989) describes the synthesis of an enzyme in a bacterial cell. Here S_{10} denotes the enzyme and S_3 is a *regulator gene*. In the beginning of the reaction only S_3, S_7 and S_8 are present. Since in Bock (1981) and Melenk *et al.* (1989) only the differential equations are given we constructed a directed graph and a bipartite graph as in Figure 2 such that these equations result. The matrix of the directed graph is

$$A = \begin{pmatrix} A_1 & & & 0 \\ & A_2 & & \\ & & A_3 & \\ 0 & & & A_4 \end{pmatrix}$$

with

$$A_1 = \left[\begin{array}{ccc|c} -p_2 - p_3 & 0 & p_1 & 0 \\ 0 & -p_4 & p_{15} & 0 \\ p_2 & p_4 & -p_1 - p_{15} & 0 \\ \hline p_3 & 0 & 0 & 0 \end{array}\right], \qquad A_2 = \left[\begin{array}{cccc|c} -p_{12} & 0 & 0 & 0 & 0 \\ p_{12} & -p_7 & 0 & 0 & 0 \\ 0 & p_7 & -p_6 & 0 & 0 \\ 0 & 0 & p_6 & -p_8 & 0 \\ \hline 0 & 0 & 0 & p_8 & 0 \end{array}\right],$$

$$A_3 = \left[\begin{array}{ccc|c|c} -p_{13} & 0 & 0 & 0 & 0 \\ 0 & -p_{11} & p_{10} & 0 & 0 \\ p_{13} & 0 & -p_{10} - p_{14} & 0 & 0 \\ \hline 0 & p_{11} & 0 & 0 & 0 \\ \hline 0 & 0 & p_{14} & 0 & 0 \end{array}\right], \qquad A_4 = \left[\begin{array}{cc|c} -p_5 & 0 & 0 \\ 0 & -p_9 & 0 \\ \hline p_5 & p_9 & 0 \end{array}\right].$$

The index sets of the connected components and of the terminal strong connected components of the weighted directed graph are

$$\begin{array}{llll} \mathcal{L}_1 = \{1,2,3,4\}, & \mathcal{T}_1^1 = \{4\}, & \mathcal{L}_2 = \{5,6,7,8,9\}, & \mathcal{T}_2^1 = \{9\}, \\ \mathcal{L}_3 = \{10,11,12,13,14\}, & \mathcal{T}_3^1 = \{13\}, \mathcal{T}_3^2 = \{14\}, & \mathcal{L}_4 = \{15,16,17\}, & \mathcal{T}_4^1 = \{17\}. \end{array}$$

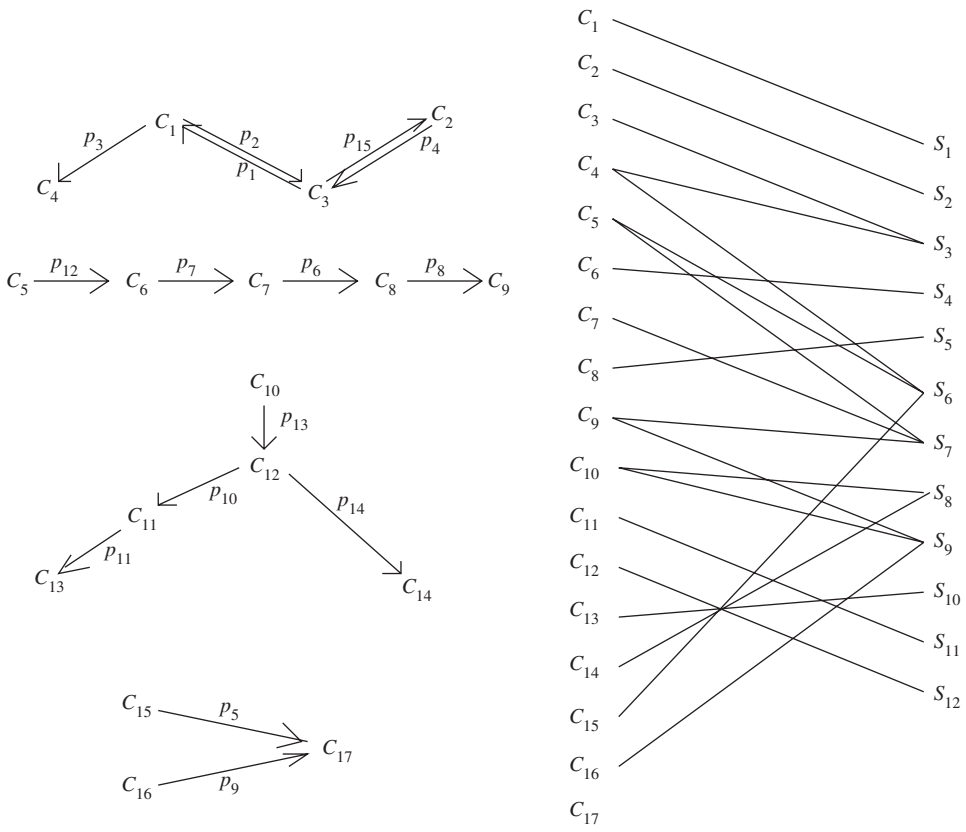

Figure 2. Enzyme synthesis in a bacterial cell (Heinmets). In the bipartite graph on the right we assume the convention that a weight of the edge $C_j - S_i$ is $y_{ij} = 1$ if no number is drawn. If C_j and S_i are not adjacent then $y_{ij} = 0$. The weights p_i in the directed graph on the left are all positive constants.

The described differential equations with positive constants p_i are

$$\begin{aligned}
\dot{x}_1 &= (-p_2 - p_3)x_1 + p_1 x_3 & \dot{x}_2 &= -p_4 x_2 + p_{15} x_3 \\
\dot{x}_3 &= (p_2 + p_3)x_1 + p_4 x_2 - (p_1 + p_{15})x_3 & \dot{x}_4 &= p_{12} x_6 x_7 - p_7 x_4 \\
\dot{x}_5 &= p_6 x_7 - p_8 x_5 & \dot{x}_6 &= p_3 x_1 - p_{12} x_6 x_7 - p_5 x_6 \\
\dot{x}_7 &= -p_{12} x_6 x_7 + p_7 x_4 - p_6 x_7 + p_8 x_5 & \dot{x}_8 &= -p_{13} x_8 x_9 + p_{14} x_{12} \\
\dot{x}_9 &= p_8 x_5 - p_{13} x_8 x_9 - p_9 x_9 & \dot{x}_{10} &= p_{11} x_{11} \\
\dot{x}_{11} &= -p_{11} x_{11} + p_{10} x_{12} & \dot{x}_{12} &= p_{13} x_8 x_9 + p_{11} x_{11} - (p_{10} + p_{14}) x_{12}.
\end{aligned}$$

We are interested in the steady state solutions. That means $\dot{x} = 0$. Since $\operatorname{rank}(A_3) = \operatorname{rank}(Y_3 A_3) = 3$ and $\operatorname{rank}(YA) = 9$, but $\operatorname{rank}(Y_1 A_1, Y_2 A_2, Y_4 A_4) = 6$ with $Y = (Y_1, Y_2, Y_3, Y_4)$ we deduce that $A_3 \tilde{\Psi}(x) = 0$ must be satisfied. This is equivalent to the equations

$$x^{y_{10}} = x_8\, x_9 = 0, \qquad x^{y_{11}} = x_{11} = 0, \qquad x^{y_{12}} = x_{12} = 0.$$

The assumptions of Lemma 5.1 are satisfied for $i = 10, 11, 12$. Obviously, we need to consider two cases.

1. Case ($x_8 = x_{11} = x_{12} = 0$): substitution gives the remaining equations

$$\begin{aligned}(-p_2 - p_3)x_1 + p_1x_3 &= 0 & -p_4x_2 + p_{15}x_3 &= 0\\ (p_2 + p_3)x_1 + p_4x_2 + (-p_1 - p_{15})x_3 &= 0 & p_{12}x_6x_7 - p_7x_4 &= 0\\ p_6x_7 - p_8x_5 &= 0 & p_3x_1 - p_{12}x_6x_7 - p_5x_6 &= 0\\ -p_{12}x_6x_7 + p_7x_4 - p_6x_7 + p_8x_5 &= 0 & p_8x_5 - p_9x_9 &= 0.\end{aligned}$$

   These are seven linear equations in nine monomials. A solution is obviously

$$x_1 = \frac{x_6(p_{12}x_7 + p_5)}{p_3}, \quad x_3 = \frac{x_6(p_2p_{12}x_7 + p_5p_2 + p_{12}x_7p_3 + p_5p_3)}{p_3p_1}, \quad x_5 = \frac{p_6x_7}{p_8},$$
$$x_2 = \frac{p_{15}x_6(p_2p_{12}x_7 + p_5p_2 + p_{12}x_7p_3 + p_5p_3)}{p_4p_1p_3}, \quad x_4 = \frac{p_{12}x_6x_7}{p_7}, \quad x_9 = \frac{p_6x_7}{p_9}.$$

2. Case ($x_9 = x_{11} = x_{12} = 0$): this yields $x_5 = 0$, $x_7 = 0$, $x_4 = 0$ and

$$x_1 = \frac{p_5x_6}{p_3}, \qquad x_2 = \frac{p_{15}p_5x_6(p_2 + p_3)}{p_4p_1p_3}, \qquad x_3 = \frac{p_5x_6(p_2 + p_3)}{p_3p_1}.$$

These solutions have been computed in Melenk *et al.* (1989) using Gröbner bases in the ring $Q(p)[x]$. Exploiting the structure this system is easily solved by elementary linear algebra.

The proof of the Lemma 5.1 is based on the approach to first solve the linear system $YAz = 0$ and then solve $z = \Psi(x)$. The assumptions in Lemma 5.1 on the graphs yields a solution of the first system with $z_i = 0$. In turn the second system gives solutions with some $x_j = 0$. For sparse polynomial systems in general this is a non-generic situation, but for chemical reaction systems this happens easily because of the structure of the graphs. In the following this trivial situation will not show up.

6. Exploiting the Sublattice

If system (5) contains no mixed equations the lattice generated by the exponents of the monomials is known because there is a close relation between coefficients and exponents. In fact an explicit decoupling of the equations is possible by choosing an appropriate basis of the lattice (**Z**-module). For computation of a good module basis we use the Hermite normal form (Adkins and Weintraub, 1992, p. 301). For its efficient implementation see Storjohann (1998) and Storjohann and Labahn (1996). A hint to the following lemma may be found in Feinberg (1987, p. 2262).

LEMMA 6.1. *Consider the system $YA\Psi(x) = 0$ induced by the two graphs. Assume that the directed graph is weakly reversible and*

$$\operatorname{rank}(YA) = \sum_{\lambda=1}^{l} \operatorname{rank}(Y_\lambda A_\lambda), \tag{6}$$

where l denotes the number of connected components, $A = (a_{ij})_{i,j=1,\dots,n}$ and

$$A_\lambda = (a_{ij})_{i,j\in\mathcal{L}_\lambda}, \qquad Y_\lambda = (y_{ij})_{i=1,\dots,m,j\in\mathcal{L}_\lambda},$$

are collections of columns and rows corresponding to connected components, respectively.

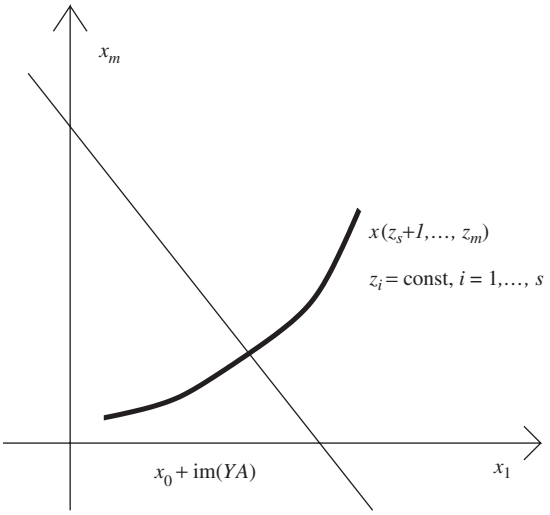

Figure 3. Transversal nonlinear parameterization derived from Hermite normal form.

By $v_i, i = 1, \ldots, m - \text{rank}(YA)$ we denote an orthonormal basis of $\ker((YA)^t)$ and consider the family of sets $\{x \in (\mathbf{R}_+)^m \mid v_i^t x - a_i = 0, i = 1, \ldots, m - \text{rank}(YA)\}$ parametrized by the constants $a_i \in \mathbf{R}$.

Then all non-empty sets of this family contain the same number of real positive solutions of $YA\Psi(x) = 0$.

Proof. Condition (6) implies that the system $YA\Psi(x) = 0$ is equivalent to

$$\sum_{j \in \mathcal{L}_\lambda} c_{ij}\, x^{y_j} = 0, \qquad i = 1, \ldots, \text{rank}(Y_\lambda A_\lambda), \qquad \lambda = 1, \ldots, l,$$

where c_{ij} are constants.

For each connected component we choose a monomial $x^{y_{j(\lambda)}}$. Since we are interested in positive solutions we may divide by this monomial and we obtain the equivalent equations

$$\sum_{j \in \mathcal{L}_\lambda \setminus \{j(\lambda)\}} c_{ij}\, x^{y_j - y_{j(\lambda)}} = -c_{ij(\lambda)}, \qquad i = 1, \ldots, \qquad \lambda = 1, \ldots, l. \tag{7}$$

In other words we shift the Newton polytopes.

Each connected component gives a sublattice generated by $y_j - y_{j(\lambda)}, j \in \mathcal{L}_\lambda \setminus \{j(\lambda)\}$. We are interested in the lattice given as the sum of these sublattices. In the matrix $YA = YI_a I_K$ the columns of YI_a are differences such as $y_j - y_i$ and I_K does not change the rank. Because of this and since the directed graph is weakly reversible the sublattice associated to $\mathcal{L}_\lambda$ has dimension $\text{rank}(Y_\lambda A_\lambda)$. Condition (6) implies that the sublattices are independent and thus the full lattice has dimension $\text{rank}(YA) = \dim(S) = s$.

We collect the differences $y_j - y_{j(\lambda)}, j \in \mathcal{L}_\lambda \setminus \{j(\lambda)\}$ as columns of a matrix Π. Then

the Hermite normal form $U\Pi = H$ with upper staircase form

$$U\Pi = \begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1l} \\ \mathbf{0} & H_{22} & \cdots & H_{2l} \\ \vdots & & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & & H_{ll} \\ \mathbf{0} & & \cdots & \mathbf{0} \end{pmatrix}$$

and unimodular U is computed. The upper staircase blocks $H_{\lambda\lambda}$ have integer entries and $\operatorname{rank}(Y_\lambda A_\lambda)$ many rows and $|\mathcal{L}_\lambda| - 1$ many columns. There are $m - s$ zero-rows. We introduce new coordinates $z = (z_1, \ldots, z_m)$ which are collected into blocks $Z_1, \ldots, Z_l, Z_{l+1}$ where Z_λ collects $\operatorname{rank}(Y_\lambda A_\lambda)$ many variables associated to the connected component λ. The remaining variables are $Z_{l+1} = (z_{s+1}, \ldots, z_m)$. The nonlinear change of coordinates $x_i = z_1^{u_{1i}} \cdots z_m^{u_{mi}}, i = 1, \ldots, m$ uses the invertible matrix $U = (u_{ij})$ giving a one-to-one-correspondence between x and z. Substitution gives new monomials in z. Denote the columns of Π by π_i and the columns of H by h_i. The monomial x^{π_i} is transformed into the monomial z^{h_i}. But H involves many zeros.

After substitution, system (7) is decoupled. The first group of $\operatorname{rank}(Y_1 A_1)$ many polynomials depends on the variables Z_1 of order $\operatorname{rank}(Y_1 A_1)$. The second group involves additionally Z_2 and so on:

$$F_1(Z_1) = 0, \qquad F_2(Z_1, Z_2) = 0, \ldots, \; F_l(Z_1, \ldots, Z_l) = 0.$$

The variables Z_{l+1} do not appear at all. That means we have an explicit parameterization by $z_{s+1}, \ldots, z_m$ of the solution variety of $YA\Psi(x) = 0$.

But we are only interested in those x which satisfy the conservation relations $v_i^t x - a_i = 0$, $i = 1, \ldots, m - s$ imposing some conditions on the remaining variables $z_{s+1}, \ldots, z_m$. Remember that $\{x \in \mathbf{R}^m \mid v_i^t x - a_i = 0 \, i = 1, \ldots, m-s\}$ equals an affine space $x_0 + \operatorname{im}(YA)$ with some appropriate x_0 with $a_i = v_i^t x_0$.

A solution $x = z^U$ is positive if and only if z is positive.

The linearization $\frac{d}{dz} x(z_{s+1}, \ldots, z_m)$ is given by

$$\frac{\partial x_j}{\partial z_i} = u_{ij} z_1^{u_{1j}} z_2^{u_{2j}} \cdots z_i^{u_{ij}-1} \cdots z_m^{u_{mj}} = u_{ij} \frac{1}{z_i} x_j \quad j = 1, \ldots, m, \; i = s+1, \ldots, m.$$

$\frac{\partial x}{\partial z_i}$ is a modification of the ith row of U which for $i = s+1, \ldots, m$ is orthogonal to $\operatorname{im}(YA) = S = \operatorname{im}(\Pi)$. If x is positive then $\operatorname{diag}(1/x_1, \ldots, 1/x_m)$ defines a weighted inner product. With respect to this local inner product $\frac{\partial x}{\partial z_i}$ is orthogonal to $\operatorname{im}(YA)$. This shows that the real positive variety is always transversal to the affine spaces $x_0 + \operatorname{im}(YA)$. Moreover, the equations $F(Z_1, \ldots, Z_l) = 0$ have finitely many solutions because they have a suitable Gröbner basis. After linear arrangements look at the leading terms with respect to the reverse lexicographic ordering. Each leading term is a support involving one additional variable. Then a Gröbner basis has this property too, yielding finitely many complex solutions. By the finiteness and the transversality each set $\{x \in (\mathbf{R}_+)^m \mid v_i^t x - a_i = 0, i = 1, \ldots, m - s\}$ contains exactly the same number of real positive solutions. □

In Lemma 6.1 we have the nice situation that the lattice is the direct sum of the sublattices associated to each connected component. The conditions in Lemma 6.1 are strong. If the directed graph is not weakly reversible or the rank condition (6) is violated then the lattice has dimension larger than $\operatorname{rank}(YA)$. Most often the dimension is m. But

in some special cases it is still possible to make statements about directions transversal to the variety using the same technique.

LEMMA 6.2. *Let the connected component $\mathcal{L}_\lambda$ equal its terminal strong connected components for some $\lambda \in \{1,\dots,l\}$ and assume*

$$\operatorname{rank}(YA) = \operatorname{rank}(Y_\lambda A_\lambda) + \operatorname{rank}(Y_1 A_1 \cdots \widehat{Y_\lambda A_\lambda} \cdots Y_l A_l), \tag{8}$$

where $\widehat{Y_\lambda A_\lambda}$ means that this block is neglected. Let v_i denote linearly independent normal vectors being orthogonal to $\operatorname{im}(YA)$. *Let w_j denote linearly independent normal vectors being orthogonal to v_i and* $\operatorname{im}(Y_\lambda A_\lambda)$. *We consider a family of non-empty sets $S_{ab} = \{x \in (\mathbf{R}_+)^m \mid v_i^t x - a_i = 0, i = 1,\dots,m - \operatorname{rank}(YA), w_j^t x - b_j, j = 1,\dots,\}$ which is parametrized by a_i and b_j. If the variety of $YA\Psi(x) = 0$ intersects a member S_{ab} of the family then it intersects transversally. All sets in the family contain the same number of positive solutions of $Y_\lambda A_\lambda \tilde{\Psi}(x) = 0$. If additionally* $\operatorname{rank}(A_\lambda) = \operatorname{rank}(Y_\lambda A_\lambda)$ *then each S_{ab} contains precisely one positive solution of $Y_\lambda A_\lambda \tilde{\Psi}(x) = 0$.*

PROOF. By the rank condition the system $YA\Psi(x) = 0$ decouples into $Y_\lambda A_\lambda \tilde{\Psi}(x) = 0, \tilde{\Psi}_i(x) = x^{y_i}, i \in \mathcal{L}_\lambda$ and some other equations. Choosing one $j(\lambda) \in \mathcal{L}_\lambda$ we divide by $x^{y_{j(\lambda)}}$ and thus have to investigate the lattice generated by $y_j - y_{j(\lambda)}, j \in \mathcal{L}_\lambda \setminus \{j(\lambda)\}$. As in the proof of the previous lemma the parameterization of the variety of $Y_\lambda A_\lambda \tilde{\Psi}(x) = 0$ is transversal to each S_{ab}.

If additionally $\operatorname{rank}(A_\lambda) = \operatorname{rank}(Y_\lambda A_\lambda)$ then $Y_\lambda A_\lambda \tilde{\Psi}(x) = 0$ is equivalent to $A_\lambda \tilde{\Psi}(x) = 0$. By Theorem 3.2 this is equivalent to a binomial system. Binomial systems have either no positive solution or precisely one positive solution. Here we have precisely one positive solution which is easily seen as follows. By Theorem 3.2 a kernel vector u of A_λ is positive. $u = \Psi(x)$ is solved by a nonlinear change of variables given by the Smith normal form or the Hermite normal form. This gives precisely one positive solution. For more details see the proof of Theorem 7.1. □

We view the solutions of the system $YA\Psi(x) = 0$ and $v_i^t x - a_i = 0, i = 1,\dots,m - \operatorname{rank}(YA)$ as the intersection of the set of the solution of $YA\Psi(x) = 0$ with the set of solutions of $v_i^t x - a_i = 0, i = 1,\dots,m - \operatorname{rank}(YA)$. Especially, we would like to know how the solutions vary if the constants a_i are varied. In general this dependency may be very complicated. In this section we investigated cases where the intersection of the two solution sets in the positive orthants are transversal. Moreover, the number of positive solutions did not depend on the choice of the constants a_i.

7. Using Toric Varieties

The proofs of the known deficiency theorems in this section are based on toric varieties, a fundamental concept which we explain first.

Suppose we are interested in the complex solutions $x \in (\mathbf{C} \setminus \{0\})^m$ of a system of sparse Laurent polynomials

$$B\,\chi(x) = 0, \qquad \chi(x) = \begin{pmatrix} x^{a_1} \\ \vdots \\ x^{a_n} \end{pmatrix} \tag{9}$$

with a matrix $B \in \mathbf{C}^{m,n}$ and support $\mathcal{A} = \{a_1, \ldots, a_n\} \subset \mathbf{Z}^m$ generating a vector space of dimension m. Then the *toric ideal* $I_{\mathcal{A}} = \{p \in \mathbf{C}[z_1, \ldots, z_n] \,|\, p(x^{a_1}, \ldots, x^{a_n}) \equiv 0\}$ defines the affine toric variety $X_{\mathcal{A}} = V(I_{\mathcal{A}}) = \{z \in \mathbf{C}^n \,|\, p(z) = 0 \ \forall p \in I_{\mathcal{A}}\}$. Each solution $x \in (\mathbf{C} \setminus \{0\})^m$ of (9) defines a $z = \chi(x) \in X_{\mathcal{A}} \cap (\mathbf{C} \setminus \{0\})^n$ in $\ker(B)$ and conversely each $z \in X_{\mathcal{A}} \cap (\mathbf{C} \setminus \{0\})^n \cap \ker(B)$ gives at least one solution $x \in (\mathbf{C} \setminus \{0\})^m$ of (9) by solving $z = \chi(x)$ with Hermite normal form. Since $\ker(B)$ is a linear vector space one better use the version with homogenized monomials: $\tilde{x} = (\tilde{x}_0, \ldots, \tilde{x}_n)$, $d = \max_{i=1,\ldots,n}(\deg(x^{a_i}))$, $\tilde{a}_i = (d - \deg(a_i), a_i)$ with monomials $\tilde{\chi}_i(\tilde{x}) = \tilde{x}^{\tilde{a}_i}$. That means we think of $\mathbf{C}^m$ as embedded in the projective space $\mathbf{P}^m$ by $x_i = \frac{\tilde{x}_i}{\tilde{x}_0}, i = 1, \ldots, m$. By changing coordinates we might as well use the support

$$\hat{\mathcal{A}} = \left\{ \begin{pmatrix} 1 \\ a_1 \end{pmatrix}, \ldots, \begin{pmatrix} 1 \\ a_n \end{pmatrix} \right\},$$

and $\hat{\chi}(\hat{x}_0, \ldots, \hat{x}_n) = (\hat{x}_0 \hat{x}^{a_1}, \ldots, \hat{x}_0 \hat{x}^{a_n})$, with monomials $\hat{\chi}_i(\hat{x}) = \hat{x}^{\hat{a}_i}$. Then the homogeneous toric ideal

$$I_{\hat{\mathcal{A}}} = \{p \in \mathbf{C}[z] \,|\, p(x_0 x^{a_1}, \ldots, x_0 x^{a_n}) \equiv 0\},$$

gives the *projective toric variety* $X_{\hat{\mathcal{A}}} = V(I_{\hat{\mathcal{A}}}) \subset \mathbf{P}^{n-1}$. Each $z \in (\mathbf{C} \setminus \{0\})^n$ with $[z] \in X_{\hat{\mathcal{A}}}$ and $Bz = 0$ gives solutions $x \in (\mathbf{C} \setminus \{0\})^m$ of (9) by solving $\hat{\chi}(\hat{x}) = z$ and setting $x_i = \hat{x}_i, i = 1, \ldots, m$.

Thus finding solutions x of (9) is equivalent to finding solutions z of

$$Bz = 0, \qquad z^{u_j} - z^{v_j} = 0, \ j = 1, \ldots$$

where $z^{u_j} - z^{v_j}$ denote a set of generators of $I_{\hat{\mathcal{A}}}$. The name toric variety comes from the fact that the rescaling $(\tilde{x}_0, t_1 \tilde{x}_1, \ldots, t_n \tilde{x}_n)$ with $t \in (\mathbf{C} \setminus \{0\})^m$ of points in the projective space $\mathbf{P}^m$ defines a group action of the torus group $T = (\mathbf{C} \setminus \{0\})^m$ which induces a torus action on $\mathbf{P}^{n-1}$. Then $X_{\hat{\mathcal{A}}}$ is invariant under T. Moreover, the orbit $\mathcal{O}_{\mathbf{1}} = \{[z] \in \mathbf{P}^{n-1} \,|\, z = (t_1^{a_{11}} \cdots t_m^{a_{1m}}, \ldots, t_1^{a_{n1}} \cdots t_m^{a_{nm}}) = t \cdot \mathbf{1}\}$ is dense and open in $X_{\hat{\mathcal{A}}}$. The rest of $X_{\hat{\mathcal{A}}} \setminus \mathcal{O}_{\mathbf{1}}$ is given by points with some coordinates $z_i = 0$ corresponding to points with some $x_j = 0$ or $1/x_j = 0$. Often toric varieties are considered in a more sophisticated manner than here (for a discussion see, for example, Chapter 13 in Sturmfels, 1996 or Gelfand *et al.*, 1994).

Restricting ourselves to positive solutions of (9) with $B \in \mathbf{R}^{m,n}$ we observe the following. Using the Hermite normal form it is easily seen that $(\mathbf{R}_+)^m$ is isomorphic to the interior of $X_{\geq 0} = \{[z] \in X_{\hat{\mathcal{A}}}, z \geq 0\}$. Thus one needs to investigate the intersection of the interior of the convex polyhedral cone $\ker(B) \cap (\mathbf{R}_{\geq 0})^n$ with $X_{\geq 0}$. The proof of the Deficiency Zero Theorem (Theorem 7.1) for one connected component fits into this principle with $X_{\hat{\mathcal{A}}} = \mathbf{P}^{n-1}$. In the Deficiency One Theorem (Theorem 7.3) the toric ideal is generated by one polynomial.

The name of the following theorem (Feinberg, 1979, 1987, also cited in Epstein and Pojman, 1998, p. 100) reflects the assumption that the deficiency $\operatorname{rank}(A) - \operatorname{rank}(YA)$ is zero.

THEOREM 7.1. (DEFICIENCY ZERO THEOREM) *Consider the system* $YA\Psi(x) = 0$ *with* $A = K - \operatorname{diag}(K^t e)$ *with* $e = (1, \ldots, 1)$ *defined by the weighted adjacency matrix* K *of a weighted directed graph and the relevant part* Y *of an adjacency matrix of a weighted bipartite graph. Let* $v_i, i = 1, \ldots, m - \operatorname{rank}(YA)$ *denote an orthonormal basis of* $\ker((YA)^t)$.

If the directed graph is weakly reversible and

$$\operatorname{rank}(A) = \operatorname{rank}(YA),$$

then each non-empty set $\{x \in (\mathbf{R}_+)^m \mid v_i^t x - a_i = 0, i = 1, \ldots, m - \operatorname{rank}(YA)\}$ *contains precisely one real positive solution of* $YA\Psi(x) = 0$.

PROOF. Since the directed graph is weakly reversible and $\operatorname{rank}(YA) = \operatorname{rank}(A)$ conditions (6) and (8) are satisfied. So the lattice is the direct sum of its sublattices and by Lemmas 6.1 and 6.2 it is sufficient to look at the case that the directed graph has one connected component which equals its terminal strong connected component.

Using the idea of toric varieties we need to solve $YAz = 0$ and investigate the toric variety. For the first task we observe that $\operatorname{rank}(YA) = \operatorname{rank}(A)$ implies that the equations $YAz = 0$ are equivalent to $Az = 0$. By Theorem 3.2 $\ker(A)$ is generated by one positive vector z since there is one weakly reversible connected component only.

The toric ideal $I_{\hat{Y}}$ is defined by the lifted monomials $\hat{x}_0 \hat{x}^{y_j}, j = 1, \ldots, n$ and we denote

$$\hat{Y} = \begin{pmatrix} 1 & \cdots & 1 \\ & Y & \end{pmatrix}.$$

$I_{\hat{Y}}$ is generated by polynomials given by kernel vectors of $\hat{Y}$ (see Chapter 4 in Sturmfels, 1996). Since we show later that $\operatorname{rank}(\hat{Y}) = n$ we have $I_{\hat{Y}} = \{0\}$ and the projective toric variety $V(I_{\hat{Y}})$ equals the projective space $\mathbf{P}^{n-1}$. The rank of $\hat{Y}$ is equal to the rank of

$$\begin{pmatrix} 1 & 0 & \cdots & 0 \\ y_1 & y_2 - y_1 & \cdots & y_n - y_1 \end{pmatrix}.$$

Since there is only one connected component being both strong and terminal we have $\operatorname{rank}(A) = \operatorname{rank}(I_a)$ and thus $\operatorname{rank}(YA) = \operatorname{rank}(YI_a) = n - 1$. Since I_a is an incidence matrix $\operatorname{rank}(YI_a)$ equals the dimension of $\operatorname{span}(y_2 - y_1, \ldots, y_n - y_1)$. Thus $\operatorname{rank}(\hat{Y}) = n$.

It remains to solve $\hat{\chi}(\hat{x}) = z$, where $\hat{\chi}_i(\hat{x}) = \hat{x}_0 \hat{x}^{y_i}$ and z is the positive vector which generates $\ker(YA)$. The Hermite normal form of $\hat{Y}$ is given by a unimodular matrix $U \in GL(m+1, m+1, \mathbf{Z})$ and an upper triangular matrix $H \in \mathbf{Z}^{m+1,n}$ with $U\hat{Y} = H$. The last $m - n + 1$ rows of H are zero by $\operatorname{rank}(\hat{Y}) = n$. The invertible matrix $U = (u_{ij})_{i,j=0,\ldots,m}$ suggests the nonlinear change of coordinates $\hat{x}_i = \prod_{j=0}^m w_j^{u_{ji}}, i = 0, \ldots, m$. This transforms $\hat{\chi}(\hat{x}) = z$ into a binomial system

$$w^{h_1} = z_1, \ldots, \qquad w^{h_n} = z_n, \tag{10}$$

where $h_1, \ldots, h_n$ denote the columns of H. Because the last rows of H are zero, system (10) does not depend on $w_n, \ldots, w_m$. Since system (10) is triangular and z is positive there is exactly one positive solution $w_0, \ldots, w_{n-1}$ of (10). Thus $w_n, \ldots, w_m$ give an explicit parametrization of the variety of $YA\Psi(x) = 0$. Here $x_i = \hat{x}_i, i = 1, \ldots, m$ and

$$\frac{dx_i}{dw_j} = u_{ji} w_0^{u_{0i}} \cdots w_j^{u_{ji}-1} \cdots w_m^{u_{mi}} = u_{ji} w_0^{u_{0i}} \cdots w_j^{u_{ji}} \cdots w_m^{u_{mi}} \frac{1}{w_j} = u_{ji} x_i \frac{1}{w_j}.$$

On the positive orthant $\operatorname{diag}(1/x_1, \ldots, 1/x_n)$ defines an inner product and $\langle dx/dw_j, v \rangle = \frac{1}{w_j} U_j^t v$ with $U_j = (u_{j1}, \ldots, u_{jm})$ the jth row of U minus the first entry. But $U_j, j = n, \ldots, m$ is orthogonal to $\operatorname{span}(y_2 - y_1, \ldots, y_n - y_1)$ since the last rows of H are zero and thus the U_j are orthogonal to $\operatorname{im}(YA)$. This means the solution variety of $YA\Psi(x) = 0$ is tranversal to each affine space $x_0 + \operatorname{im}(YA) = \{x \in \mathbf{R}^m \mid v_i^t x - a_i = v_i^t x - v_i^t x_0 = 0, i =$

$1, \ldots, m-n+1\}$ in the positive orthant. That is why each space $\{x \in (\mathbf{R}_+)^m \,|\, v_i^t x - a_i = 0, i = 1, \ldots, m-n+1\}$ has precisely one positive solution. □

An alternative proof would not use the projective space but transform $YA\Psi(x) = 0$ into a binomial system directly. For solving the binomial systems there are three methods: using the logarithm (Feinberg, 1979; Itenberg and Roy, 1996) or the Hermite normal form or the Smith normal form (Adkins and Weintraub, 1992). For efficient computation of normal forms of integer matrices see Storjohann (1996, 1998); Storjohann and Labahn (1996).

A similiar case also arises for directed graphs which are not weakly reversible.

THEOREM 7.2. *Consider the system $YA\Psi(x) = 0$ of polynomial equations defined by a directed graph with weighted adjacency matrix K and incidence matrices I_a, I_K and a bipartite graph with matrix Y and $A = I_a I_K = K - \operatorname{diag}(K^t e)$. Assume the graph has one connected component only ($l = 1$). Assume*

$$\operatorname{rank}(YA) = \operatorname{rank}(A) - 1 = n - t - 1,$$

where t is the number of terminal strong connected components and n the number of vertices of the directed graph. Moreover, assume $\dim(\operatorname{span}(\{YA_i, i \in \mathcal{T}_1^\nu\})) = |\mathcal{T}_1^\nu| - 1$ *for each $\nu = 1, \ldots, t$, where A_i denotes the ith column of A and $\mathcal{T}_1^\nu$ denotes the indices of the νth terminal strong connected component. For the rest $\mathcal{R} = \mathcal{L}_1 \setminus \bigcup_\nu \mathcal{T}_1^\nu$ assume* $\dim(\operatorname{span}(\{YA_i \,|\, i \in \mathcal{R}\})) = |\mathcal{R}| - 1$ *and that $\sum_{i\in\mathcal{R}} YA_i\alpha_i = 0$ has a strict positive solution α. Moreover, we assume*

$$\operatorname{rank}(YA) = \operatorname{rank}(YI_a) = \dim(\{y_i - y_j \,|\, i, j \in \mathcal{R} \text{ or } i, j \in \mathcal{T}_1^\nu\}). \tag{11}$$

Let $v_i, i = 1, \ldots, m-n+t+1$ denote an orthonormal basis of $\ker((YA)^t)$.

Then each non-empty set $\{x \in (\mathbf{R}_+)^m \,|\, v_i^t x - a_i = 0, i = 1, \ldots, m-n+t+1\}$ contains precisely one positive real solution of $YA\Psi(x) = 0$.

PROOF. We follow the principle of intersecting a projective toric variety with the kernel of the coefficient matrix as explained at the beginning of this section. By the rank assumption rank $\ker(YA)$ has a basis $b_0, \ldots, b_t$. By Theorem 3.2 and the explicit assumptions we may assume $b_\nu \geq 0, \nu = 0, \ldots, t$ and

$$(b_0)_j = 0,\ j \in \bigcup_{i=1}^{t} \mathcal{T}_1^i, \qquad (b_\nu)_j = 0,\ j \in \mathcal{R} \cup \bigcup_{i=1, i\neq\nu}^{t} \mathcal{T}_1^i, \qquad \nu = 1, \ldots, t$$

and $\prod_{j\in\mathcal{R}}(b_0)_j \cdot \prod_{\nu=1}^{t} \prod_{j\in\mathcal{T}_1^\nu}(b_\nu)_j \neq 0$. Since the kernel vectors b_ν have disjoint support it is appropriate to look at multi-homogeneous toric ideals. Using extra variables $\hat{x}_0, \hat{x}_{01}, \ldots, \hat{x}_{0t}$ we define *homogenized* monomials

$$\hat{\psi}_j(\hat{x}) = \begin{cases} \hat{x}_0 \hat{x}_{0\nu} \hat{x}^{y_j}, & \text{if } j \in \mathcal{T}_1^\nu \text{ for one } \nu \in \{1, \ldots, t\}, \\ \hat{x}_0 \hat{x}^{y_j} & \text{if } j \in \mathcal{R}, \end{cases} \qquad j = 1, \ldots, n.$$

By this construction a solution $\hat{x}$ which is determined from the intersection of $\ker(YA)$ with the toric variety gives the solution $x_j = \hat{x}_j, j = 1, \ldots, m$. The toric ideal is generated by polynomials derived from kernel vectors of $\hat{Y}$ whose jth column is formed by the exponents of $\hat{\psi}_j$. The rank of $\hat{Y}$ is $1 + t + \dim(\{y_i - y_j \,|\, i, j \in \mathcal{R} \text{ or } i, j \in \mathcal{T}_1^\nu\})$. The

desired dimension is by assumption $n-t-1$. Then $\operatorname{rank}(\hat{Y}) = n$ and the toric variety is a product of projective spaces.

Now one solves $\hat{\psi}(\hat{x}) = \sum_{\nu=0}^{t} \lambda_\nu b_\nu$. Once more we use the Hermite normal form $U\hat{Y} = H$ and a nonlinear change of coordinates. Since for each j there is a ν with $(b_\nu)_j > 0$ there is precisely one positive solution, but some variables remain arbitrary. There is a parametrization of the solutions of $YA\psi(x) = 0$ by $m-n$ slack variables $w_1, \ldots, w_{m-n}$. (Observe that $x(w_1, \ldots, w_{m-n})$ does not depend on λ_ν.) As in the proof of the Deficiency Zero Theorem this variety is in the positive orthant transversal to each space $\{x \in (\mathbf{R}_+)^m \,|\, v_i^t x - a_i = 0\}$ by use of the local inner product and the fact that the last rows of U are orthogonal to the lattice. It is here where we require condition (11). □

Condition (11) makes an explicit assumption on the lattice. In Lemmas 6.1 and 6.2 and the deficiency theorems there are no explicit assumptions on the lattice since the assumptions on the coefficient matrix YA imply conditions for the lattice.

In Feinberg (1979, 1987, 1988), Feinberg formulates a theorem which he calls the *Deficiency One Theorem* since a rank defect is one. The assumptions in Feinberg (1988) are more restrictive than in Feinberg (1979). We present our version here. This theorem should not be confused with the deficiency one theorem in Feinberg (1995b) which makes different assumptions leading to several positive solutions.

Theorem 7.3. (Deficiency One Theorem, Feinberg, 1987 p. 2259, proof in Feinberg, 1995a) *Let the graph be weakly reversible and* $\operatorname{rank}(Y_\lambda A_\lambda) \geq |\mathcal{L}_\lambda| - 2$ *for each connected component, where* $\lambda = 1, \ldots, l$. *Moreover, assume*

$$\operatorname{rank}(YA) = \sum_{\lambda=1}^{l} \operatorname{rank}(Y_\lambda A_\lambda). \tag{12}$$

Let $v_i, i = 1, \ldots, m - \operatorname{rank}(YA)$ *denote an orthonormal basis of* $\ker((YA)^t)$.

Then each non-empty set $\{x \in (\mathbf{R}_+)^m \,|\, v_i^t x - a_i = 0, i = 1, \ldots, m - \operatorname{rank}(YA)\}$ *contains precisely one real positive solution of the polynomial equations* $YA\Psi(x) = 0$.

Proof. Because of assumption (12) on the rank, the polynomial system decouples as stated in the proof of Lemma 6.1. Consequently, we restrict ourselves to the case where the graph has one connected component with $\operatorname{rank}(YA) = \operatorname{rank}(A) - 1 = n-2$. Moreover, the nonlinear change of coordinates decouples the equations $YA\Psi(x) = 0$ and the linear conservation relations. As in the proof of Lemma 6.1 each space $(x_0 + \operatorname{im}(YA)) \cap (\mathbf{R}_+)^m = \{x \in \mathbf{R}_+)^m \,|\, v_i^t x - v_i^t x_0 = 0, i = 1, \ldots\}$ contains the same number of positive solutions. It remains to show the existence of precisely one solution.

First we like to find generators of the convex polyhedral cone $\ker(YA) \cap (\mathbf{R}_{\geq 0})^n$. By Theorem 3.2 $\operatorname{rank}(A) = n-1$ and there exist $a \in (\mathbf{R}_+)^n$ with $\ker(A) = \operatorname{span}(a)$. By assumption $\operatorname{rank}(YA) = n-2$ and thus there exist vectors $b \in (\mathbf{R}_{\geq 0})^n$ and $c \in (\mathbf{R}_{\geq 0})^n$ with zero components such that $\ker(YA) \cap (\mathbf{R}_{\geq 0})^n = \{\lambda b + \mu c \,|\, \lambda, \mu \geq 0\}$. Let us assume b has one zero component b_j and c has the zero component c_k, respectively.

Secondly, we investigate the positive part of the projective toric variety. The support $\mathcal{A} = \{y_1, \ldots, y_n\}$ gives rise to a lattice generated by $y_2 - y_1, \ldots, y_n - y_1$ of dimension $< m$. The Hermite normal form may be used to decrease the number of variables. But this does not affect the projective toric variety.

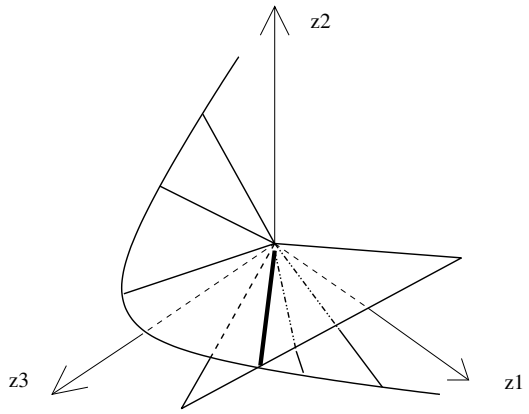

Figure 4. Schematic picture illustrating the proof of Theorem 7.3: intersection of a projective toric variety (here a hypersurface) with the kernel in $(\mathbf{R}_+)^n$, a convex polyhedral cone.

Since the connected component of the directed graph contains exactly one terminal strong connected component $\operatorname{rank}(A) = \operatorname{rank}(I_a)$, thus $\operatorname{rank}(YA) = \operatorname{rank}(YI_a)$. By assumption $\operatorname{rank}(YA) = \operatorname{rank}(YI_a) = n - 2$. Because the directed graph is weakly reversible $\operatorname{rank}(YI_a)$ equals $\dim(\operatorname{span}\{y_2 - y_1, \ldots, y_n - y_1\})$. Thus we know that the lifted support

$$\hat{\mathcal{A}} = \left\{ \begin{pmatrix} 1 \\ y_1 \end{pmatrix}, \ldots, \begin{pmatrix} 1 \\ y_n \end{pmatrix} \right\}$$

generates a vector space of dimension $n - 1$. Thus $\ker(Y) \cap \ker(\mathbf{1})$ is generated by one vector $g \in \mathbf{C}^n$ which may be chosen to be an integer whose components are relative prime.

Then $I_{\hat{\mathcal{A}}} = \langle z^{g_+} - z^{g_-} \rangle$ where

$$(g_+)_i = \begin{cases} g_i & \text{for} \quad g_i > 0 \\ 0 & \text{else} \end{cases}, \qquad (g_-)_i = \begin{cases} -g_i & \text{for} \quad g_i < 0 \\ 0 & \text{else} \end{cases}.$$

It remains to prove that there is precisely one one-dimensional intersection of $\ker(YA)$ and $X_{\geq 0}$. This means we study the behavior of $f(z) = z^{g_+} - z^{g_-}$ (or $F(z) = z^g - 1$, respectively) on the cone $\{\lambda b + \mu c \,|\, \lambda, \mu \geq 0\}$. Thus we investigate $h(\lambda, \mu) = f(\lambda b + \mu c)$. Since f is homogeneous of zero degree $h(w\lambda, w\mu) = h(\lambda, \mu)$ and we may use a scaling of (λ, μ). We will investigate $p(\lambda) = h(\lambda, 1 - \lambda)$ for $\lambda \in [0, 1]$ and show $p(1)p(0) < 0$.

In order to do so we investigate the degrees in λ and μ of the Laurent polynomial $(\lambda b + \mu c)^g$. For this we need to take into account that some components of b, c are zero. Let $\omega_{\operatorname{supp}(b)} = \sum_{i \in \operatorname{supp}(b)} \omega_i$ and $\omega_{\operatorname{supp}(c)} = \sum_{i \in \operatorname{supp}(c)} \omega_i$ be vectors with entry one for each index of the support. Then

$$\begin{aligned} \deg_\lambda((\lambda b + \mu c)^g) &= \omega_{\operatorname{supp}(b)} \cdot g, \\ \deg_\mu((\lambda b + \mu c)^g) &= \omega_{\operatorname{supp}(c)} \cdot g. \end{aligned}$$

On the other hand there exist ξ_b, ξ_c with $\xi_b g = Ab$ and $\xi_c g = Ac$. By construction the values ξ_b and ξ_c have opposite sign. Now

$$\xi_b \deg_\lambda((\lambda b + \mu c)^g) = \xi_b \left(\omega_{\operatorname{supp}(b)}\right)^t \cdot g = \left(\omega_{\operatorname{supp}(b)}\right)^t Ab,$$

which yields $\omega_{\mathrm{supp}(b)} Ab = (- \cdots - *_j - \cdots -)\ b < 0$, because A is negative diagonal dominant. Analogously, $\xi_c \deg_\mu((\lambda b + \mu c)^g) < 0$, which shows that λ and μ have different degrees in $(\lambda b + \mu c)^g$ of opposite sign (see Feinberg, 1995a, Lemma 8.1.4). Since only the change of sign matters we assume $\deg_\lambda((\lambda b + \mu c)^g) > 0$ and $\deg_\mu((\lambda b + \mu c)^g) < 0$ for simplicity of notation. Then

$$\deg_\lambda((\lambda b + \mu c)^{g_+}) > \deg_\lambda((\lambda b + \mu c)^{g_-}),$$
$$\deg_\mu((\lambda b + \mu c)^{g_+}) < \deg_\mu((\lambda b + \mu c)^{g_-}).$$

This yields

$$p(1) = h(1,0) = f(b) = b^{g_+} - b^{g_-} = b^{g_+} - b_j^{(g_-)_j} \cdots = b^{g_+} - 0 > 0,$$
$$p(0) = h(0,1) = f(c) = c^{g_+} - c^{g_-} = c_k^{(g_+)_k} \cdots - c^{g_-} = 0 - c^{g_-} < 0.$$

The polynomial $p(\lambda) \in \mathbf{R}[\lambda]$ changes sign in $[0,1]$ and thus has a zero. This shows the existence of at least one 1D intersection of $X_{\geq 0}$ with $\ker(YA)$. There is at most one 1D intersection because otherwise between two intersections the tangent space of the toric variety would include a direction parallel to $\ker(YA)$ which is impossible.

The proof uses the fact that both b and c have precisely one component being zero. In case b (or c, respectively) has several components being zero such that $b^{g_+} \gneqq 0, b^{g_-} = 0$ (or $c^{g_+} = 0, c^{g_-} \gneqq 0$, respectively) nothing changes in the proof. But a case with $g_i \cdot g_j < 0$ and $b_i = b_j = 0, i \neq j$ leads to a contradiction because there exists $\alpha \in \mathbf{R}$ with $Ab = \alpha g$ and A is negative diagonal dominant. □

This proof nicely reflects the standard techniques for investigation of sparse polynomial systems. Our case is especially simple since the toric variety is defined by one polynomial $u^{g_+} - u^{g_-}$. This gives a symbolic–numeric algorithm.

ALGORITHM 7.4. (*Compute unique positive solution reliably*)

Input: $Y \in (\mathbf{Z}_{\geq 0})^{m,n}, K \in (\mathbf{R}_{\geq 0})^{n,n}$, *constants* a_i

Assumption: *The directed graph is weakly reversible and has one component.*
$$\mathrm{rank}(YA) = \mathrm{rank}(A) - 1$$

Output: *Unique positive solution* x *of* $YA\Psi(x) = 0,\ \ v_i^t x - a_i = 0$

(*1*) *compute the generator* $z^{g_+} - z^{g_-}$ *of toric ideal by Hermite normal form or Gröbner bases,*

(*2*) *compute the minimal generators* b, c *of the cone* $\ker(YA) \cap (\mathbf{R}_{\geq 0})^n$,

(*3*) *find the solution* $\tilde{\lambda} \in [0,1]$ *of*

$$p(\lambda) = (\lambda b + (1-\lambda)c)^{g_+} - (\lambda b + (1-\lambda)c)^{g_-} = 0$$

explicitly or by numerical bisection, set $\tilde{z} = \tilde{\lambda} b + (1 - \tilde{\lambda}) c \in (\mathbf{R}_{\geq 0})^n$,

(*4*) *compute Hermite normal form* $U\hat{Y} = H$ *where* $\hat{Y} = \begin{pmatrix} \mathbf{1} \\ Y \end{pmatrix}$ *and* U *is unimodular, solve* $w^H = \tilde{z}$ *giving values* $\tilde{w}_1, \ldots, \tilde{w}_{s+1}$*, where* $w_{s+2}, \ldots, w_{m+1}$ *remain arbitrary, with* $\hat{x} = (x_0, x_1, \ldots, x_m)$ *the transformation* $\hat{x} = w^U$ *gives monomial expressions* $x_j = g_j(w_{s+1}, \ldots, w_{m+1}; \tilde{w}_1, \ldots, \tilde{w}_{s+1}), j = 1, \ldots, m$,

(*5*) *compute vectors* $v_i, i = 1, \ldots, m-s$ *orthogonal to* $\mathrm{im}(YA)$*, solve conservation relations* $v_i^t x - a_i = v_i^t g(w) - a_i = h_i(w_{s+1}, \ldots, w_{m+1}) = 0$*, for example, by numerical pathfollowing from* $\lambda_i = 0$ *to* $\lambda_i = a_i$*, compute* $\hat{x} = w^U$ *giving the solutions* $x_j = \hat{x}_j$, $j = 1, \ldots, m$.

Example 7.5. The theorem is illustrated by Example 3D1 in Feinberg (1979, pp. 3–29). We recall the directed graph and the bipartite graph in Figure 5. The equations are

$$\begin{aligned}
\dot{x}_1 &= -2\,k_{2,1}{x_1}^2 + (2\,k_{1,2} + k_{3,2})x_2 + (-k_{2,3} - k_{4,3})x_1x_3 + k_{3,4}{x_3}^2 \\
&\quad + (-k_{7,6} - k_{8,6})x_1x_4 + k_{6,7}x_5 + k_{6,8}x_6 \\
\dot{x}_2 &= k_{2,1}{x_1}^2 + (-k_{1,2} - k_{3,2} - k_{4,2})x_2 + k_{2,3}x_1x_3 + k_{2,4}{x_3}^2 \\
\dot{x}_3 &= (k_{3,2} + 2\,k_{4,2})x_2 + (-k_{2,3} + k_{4,3})x_1x_3 + (-k_{3,4} - 2\,k_{2,4} - 2\,k_{5,4}){x_3}^2 \\
&\quad + 2\,k_{4,5}x_4 - k_{10,9}x_3x_5 + k_{9,10}{x_7}^2 \\
\dot{x}_4 &= k_{5,4}{x_3}^2 - k_{4,5}x_4 + (-k_{7,6} - k_{8,6})x_1x_4 + k_{6,7}x_5 + k_{6,8}x_6 \\
\dot{x}_5 &= k_{7,6}x_1x_4 + (-k_{6,7} - k_{8,7})x_5 + k_{7,8}x_6 - k_{10,9}x_3x_5 + k_{9,10}{x_7}^2 \\
\dot{x}_6 &= k_{8,6}x_1x_4 + k_{8,7}x_5 + (-k_{6,8} - k_{7,8})x_6 \\
\dot{x}_7 &= 2\,k_{10,9}x_3x_5 - 2\,k_{9,10}{x_7}^2.
\end{aligned}$$

The weakly reversible graph has three connected components such that the blocks of YA do not interact and $\mathrm{rank}(Y_1A_1) = 3 < 4 = \mathrm{rank}(A_1)$, $\mathrm{rank}(Y_2A_2) = 2$, and $\mathrm{rank}(Y_3A_3) = 1$, where as usual $Y = (Y_1, Y_2, Y_3)$ and $A = \mathrm{diag}(A_1, A_2, A_3)$.

Since we are interested in steady state solutions we set $\dot{x} = 0$ and perform linear manipulations yielding the equations

$$\begin{aligned}
-k_{2,1}{x_1}^2 + (k_{1,2} - k_{4,2})x_2 - k_{4,3}x_1x_3 + (k_{3,4} + k_{2,4}){x_3}^2 &= 0, \\
(k_{3,2} + 2\,k_{4,2})x_2 + (-k_{2,3} + k_{4,3})x_1x_3 + (-k_{3,4} - 2\,k_{2,4}){x_3}^2 &= 0, \\
k_{5,4}{x_3}^2 - k_{4,5}x_4 &= 0,
\end{aligned}$$

for the first connected component and

$$\begin{aligned}
(-k_{7,8}k_{7,6} - k_{7,8}k_{8,6} - k_{6,8}k_{7,6})x_1x_4 + (k_{6,7}k_{6,8} + k_{6,7}k_{7,8} + k_{6,8}k_{8,7})x_5 &= 0, \\
(-k_{8,7}k_{7,6} - k_{8,7}k_{8,6} - k_{6,7}k_{8,6})x_1x_4 + (k_{6,7}k_{6,8} + k_{6,7}k_{7,8} + k_{6,8}k_{8,7})x_6 &= 0
\end{aligned}$$

for the second connected component and $k_{10,9}x_3x_5 - k_{9,10}{x_7}^2 = 0$ for the third, respectively. The monomials are clearly arranged into three groups. Moreover the three sublattices are decoupled such that no nonlinear change of coordinates by Hermite normal form is necessary. Once a solution (x_1, x_2, x_3, x_4) of the first set of equations and the conservation relation is known the other components are given by

$$x_5 = \frac{(k_{7,8}k_{7,6} + k_{6,8}k_{7,6} + k_{7,8}k_{8,6})x_1x_4}{k_{6,7}k_{6,8} + k_{6,7}k_{7,8} + k_{6,8}k_{8,7}}, \qquad x_6 = \frac{(k_{8,7}k_{7,6} + k_{8,7}k_{8,6} + k_{6,7}k_{8,6})x_1x_4}{k_{6,7}k_{6,8} + k_{6,7}k_{7,8} + k_{6,8}k_{8,7}},$$

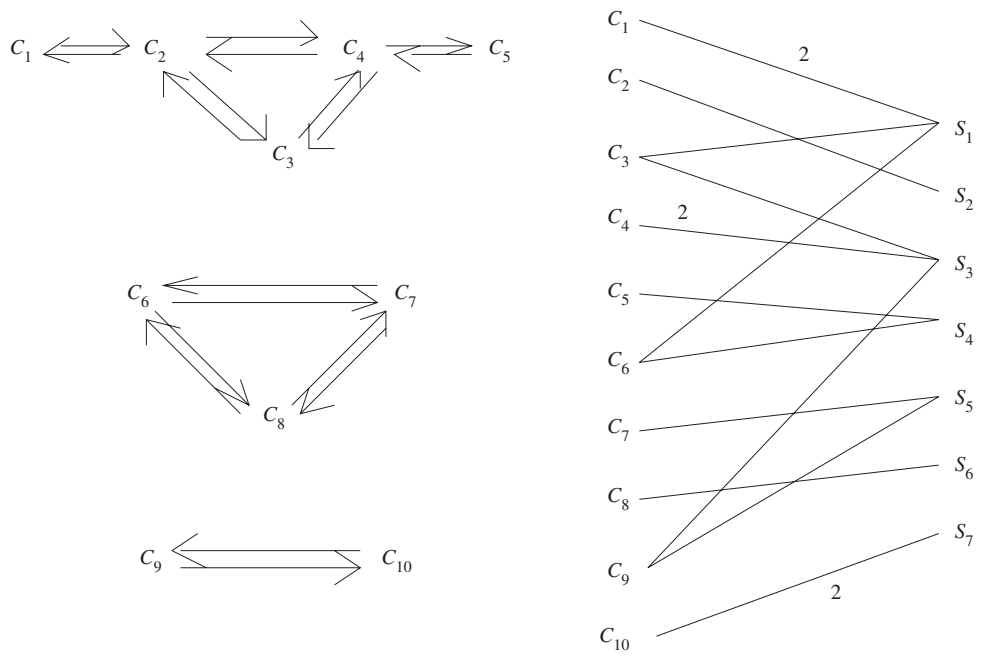

Figure 5. Example 3D1 by Feinberg.

from the second set of equations and

$$x_7 = \pm \frac{\sqrt{k_{9,10}k_{10,9}x_3x_5}}{k_{9,10}},$$

from the third connected component.

We investigate the first connected component by Algorithm 7.4. In the first step we find the vector

$$g = [1, 0, -2, 1, 0]$$

with $Y_1 g = 0$ and $\mathbf{1}^t g = 0$ which is an integer and relatively prime. Thus $f(z_1, \ldots, z_5) = z_1^1 z_4^1 - z_3^2$ is homogeneous and satisfies $f(x_1^2, x_2, x_1x_3, x_3^2, x_4) \equiv 0$.

In the second step we determine the minimal generators of the cone $\ker(YA) \cap (\mathbf{R}_{\geq 0})^5$.

$$a = \left[1, \frac{k_{2,1}}{k_{1,2}}, \frac{k_{3,4}k_{2,1}k_{4,2}}{k_{4,3}k_{2,4}k_{1,2}}, \frac{k_{2,1}k_{4,2}}{k_{2,4}k_{1,2}}, \frac{k_{5,4}k_{2,1}k_{4,2}}{k_{4,5}k_{2,4}k_{1,2}}\right],$$

generates $ker(A_1)$. We find a vector d with $g = A_1 d$ and find linear combinations with zero components yielding

$$b = \left[\frac{k_{1,2}k_{3,4} + k_{3,4}k_{4,2} + k_{2,4}k_{3,2} + 2\,k_{1,2}k_{2,4} + k_{3,4}k_{3,2}}{(k_{3,2} + 2\,k_{4,2})k_{2,1}}, \frac{k_{3,4} + 2\,k_{2,4}}{k_{3,2} + 2\,k_{4,2}}, 0, 1, \frac{k_{5,4}}{k_{4,5}}\right]$$

$$c_1 = \left[-\frac{-k_{1,2}k_{2,3} + k_{2,3}k_{4,2} + k_{4,3}k_{4,2} + k_{4,3}k_{3,2} + k_{1,2}k_{4,3}}{(k_{3,2} + 2\,k_{4,2})k_{2,1}}, -\frac{-k_{2,3} + k_{4,3}}{k_{3,2} + 2\,k_{4,2}}, 1, 0, 0\right]$$

$$c_2 = \left[0, \frac{k_{2,3}k_{2,4} + k_{2,3}k_{3,4} + k_{4,3}k_{2,4}}{k_{1,2}k_{3,4} + k_{3,4}k_{4,2} + k_{2,4}k_{3,2} + 2\,k_{1,2}k_{2,4} + k_{3,4}k_{3,2}}, 1,\right.$$

$$\frac{-k_{1,2}k_{2,3}+k_{2,3}k_{4,2}+k_{4,3}k_{4,2}+k_{4,3}k_{3,2}+k_{1,2}k_{4,3}}{k_{1,2}k_{3,4}+k_{3,4}k_{4,2}+k_{2,4}k_{3,2}+2\,k_{1,2}k_{2,4}+k_{3,4}k_{3,2}},$$
$$\frac{k_{5,4}(-k_{1,2}k_{2,3}+k_{2,3}k_{4,2}+k_{4,3}k_{4,2}+k_{4,3}k_{3,2}+k_{1,2}k_{4,3})}{(k_{1,2}k_{3,4}+k_{3,4}k_{4,2}+k_{2,4}k_{3,2}+2\,k_{1,2}k_{2,4}+k_{3,4}k_{3,2})k_{4,5}}\Bigg].$$

Then the polyhedral cone is generated by b, c_1 or b, c_2 depending on the sign of the expression $-k_{1,2}k_{2,3}+k_{2,3}k_{4,2}+k_{4,3}k_{4,2}+k_{4,3}k_{3,2}+k_{1,2}k_{4,3}$. In both cases the polynomial $p(\lambda)$ is quadratic and Maple gives the solution explicitly, but it is too complicated to present here. Consequently, the vector z is a very complicated expression. (Observe that z is not unique and only determined up to scaling.)

Now we solve $x_0x_1^2 = z_1, x_0x_2 = z_2, x_0x_1x_3 = z_3, x_0x_3^2 = z_4, x_0x_4 = z_5$ by computing the Hermite normal form $U\hat{Y}_{11} = H$ with

$$\begin{pmatrix}\mathbf{1}\\ Y_{11}\end{pmatrix} = \begin{bmatrix}1&1&1&1&1\\2&0&1&0&0\\0&1&0&0&0\\0&0&1&2&0\\0&0&0&0&1\end{bmatrix} U = \begin{bmatrix}-1&1&1&0&1\\0&0&1&0&0\\2&-1&-2&0&-2\\0&0&0&0&1\\-2&1&2&1&2\end{bmatrix} H = \begin{bmatrix}1&0&0&-1&0\\0&1&0&0&0\\0&0&1&2&0\\0&0&0&0&1\\0&0&0&0&0\end{bmatrix}.$$

U gives the transformation $x_0 = \frac{{w_3}^2}{w_1{w_5}^2}, x_1 = \frac{w_1w_5}{w_3}, x_2 = \frac{w_1w_2{w_5}^2}{{w_3}^2}, x_3 = w_5, x_4 = \frac{w_1w_4{w_5}^2}{{w_3}^2}$. From H we deduce a system in w with solution $w_1 = z_1, w_2 = z_2, w_3 = z_3, w_4 = z_5$, where w_5 is still arbitrary. This gives the solution

$$x_1 = \frac{z_1w_5}{z_3}, \qquad x_2 = \frac{z_1z_2{w_5}^2}{{z_3}^2}, \qquad x_3 = w_5, \qquad x_4 = \frac{z_1z_5{w_5}^2}{{z_3}^2}.$$

The conservation relation $v_1^t x - a_1 = 0$ determines the unknown w_5. Here

$$v_1 = [1, 2, 1, 2, 3, 3, 2],$$

which gives the equation

$$3\,\frac{{z_1}^2z_5(k_{7,8}k_{7,6}+k_{6,8}k_{7,6}+k_{7,8}k_{8,6}+k_{8,7}k_{7,6}+k_{8,7}k_{8,6}+k_{6,7}k_{8,6})}{(k_{6,7}k_{6,8}+k_{6,7}k_{7,8}+k_{6,8}k_{8,7}){z_3}^3}{w_5}^3$$
$$+\,2\left(\sqrt{\frac{k_{10,9}(k_{7,8}k_{7,6}+k_{6,8}k_{7,6}+k_{7,8}k_{8,6})z_5}{k_{9,10}{z_3}^3(k_{6,7}k_{6,8}+k_{6,7}k_{7,8}+k_{6,8}k_{8,7})}}+\frac{z_5+z_2}{{z_3}^2}\right)z_1{w_5}^2$$
$$+\left(\frac{z_1}{z_3}+1\right)w_5-a_1=0,$$

which clearly has precisely one positive solution w_5 depending on $a_1 > 0$.

All three theorems of this section use the principle that a projective toric variety is intersected with the kernel of the coefficient matrix. The projective toric variety is either a projective space or a hypersurface. The three cases may appear simultaneously in a single system (3). If condition (6) holds, and for each connected component the assumptions of one of the three theorems are satisfied, then one unique positive solution exists.

8. The General Case

In this section we apply a general theory to general system (5). If the conditions of Lemma 6.1 are fulfilled, the system decouples. So we may assume we already have

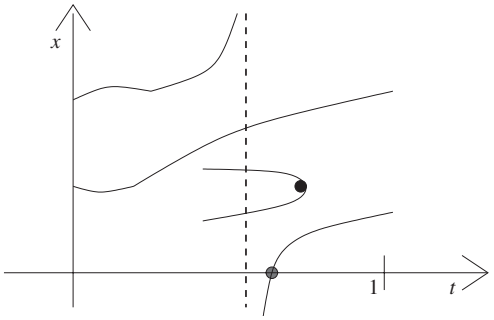

Figure 6. The number of positive solutions in the beginning ($t = 0$) of the homotopy equals the number of positive solutions in the end ($t = 1$) except if one of the three shown phenomena happens.

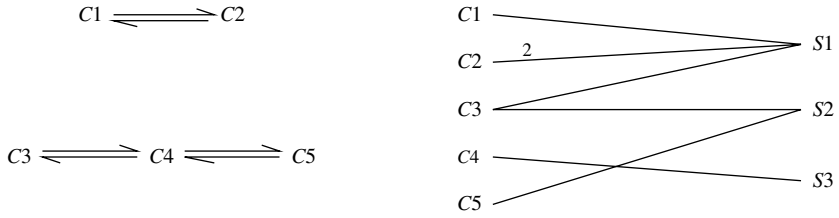

Figure 7. Example of a chemical reaction network by Feinberg due to Edelstein.

performed the decoupling and assume

$$\operatorname{rank}(Y_\lambda A_\lambda) < \operatorname{rank}(YA) - \operatorname{rank}(Y_1 A_1 \cdots \widehat{Y_\lambda A_\lambda} \cdots Y_l A_l),$$

for all $\lambda = 1, \ldots, l$. This means all connected components contribute with monomials to the middle set of mixed equations in (5).

The results on the number of complex or real solutions of a sparse polynomial system are based on a *homotopy* $\mathcal{H}(t, x)$ such that the solutions of $\mathcal{H}(0, x)$ are easily determined by solving binomial systems and $\mathcal{H}(1, x)$ is our system of interest.

$$\mathcal{H}(t,x)_{\lambda,i} = \sum_{j \in \mathcal{L}_\lambda} c_{ij}\, t^{\omega_j^\lambda} x^{y_j} = 0, \quad i = 1, \ldots, k_\lambda, \quad \lambda = 1, \ldots, l, \tag{13}$$

$$\mathcal{H}(t,x)_{l+1,i} = \sum_{j=1}^{n} b_{ij}\, t^{\omega_j^{l+1}} x^{y_j} = 0, \quad i = 1, \ldots, k_{l+1}, \tag{14}$$

$$\mathcal{H}(t,x)_{l+2,i} = \sum_{j=1}^{m} (v_i)_j\, t^{\omega_j^{l+2}} x_j - a_i t^{\omega_0^{l+2}} = 0. \quad i = 1, \ldots, k_{l+2}. \tag{15}$$

The exponents ω_j^λ are randomly chosen integer numbers. By this construction the supports of the original polynomials $\mathcal{A} = (\mathcal{A}_1, \ldots, \mathcal{A}_{l+2})$, $\mathcal{A}_\lambda = \{y_j, j \in \mathcal{L}_\lambda\}, \lambda = 1, \ldots, l$, $\mathcal{A}_{l+1} = \{y_1, \ldots, y_n\}, \mathcal{A}_{l+2} = \{0, e_1, \ldots, e_m\}$ are lifted in one additional direction giving the new supports of $\mathcal{H}$

$$\hat{\mathcal{A}}_\lambda = \left\{ \begin{pmatrix} y_j \\ \omega_j^\lambda \end{pmatrix}, j \in \mathcal{L}_\lambda \right\}, \qquad \lambda = 1, \ldots, l,$$

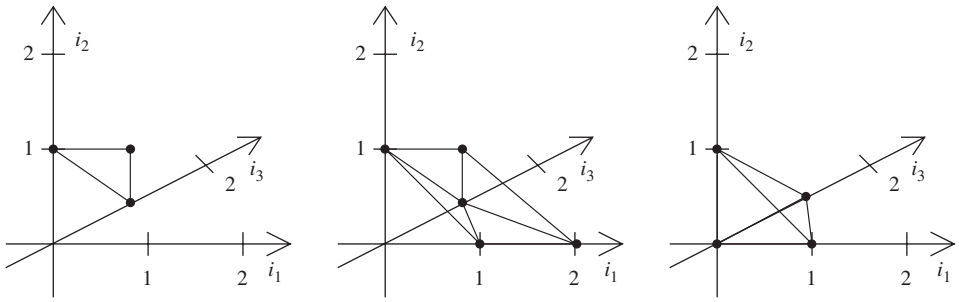

Figure 8. Newton polytopes of the system by Edelstein, where i_1, i_2, i_3 are the exponents in the monomial $x_1^{i_1} x_2^{i_2} x_3^{i_3}$.

$$\hat{\mathcal{A}}_{l+1} = \left\{ \begin{pmatrix} y_j \\ \omega_j^{l+1} \end{pmatrix}, j = 1, \ldots, n \right\}, \quad \hat{\mathcal{A}}_{l+2} = \left\{ \begin{pmatrix} 0 \\ \omega_0^{l+2} \end{pmatrix}, \begin{pmatrix} e_j \\ \omega_j^{l+2} \end{pmatrix}, j = 1, \ldots, m \right\}.$$

The lower facets of the Minkowski sum of the lifted Newton polytopes have a special meaning. They give rise to a mixed subdivision, a generalization of triangulation.

Definition. (Huber and Sturmfels, 1995; Verschelde and Gatermann, 1995; Verschelde *et al.*, 1996)

(i) A *subdivision* of $\mathcal{A} = (\mathcal{A}_1, \ldots, \mathcal{A}_{l+2})$ is a collection $\mathcal{S} = \{C_1, \ldots, C_r\}$ of r cells $C_j = (C_j^{(1)}, \ldots, C_j^{(l+2)})$ such that

  (a) $\dim(\mathrm{conv}(C_j)) = m$ for $j = 1, \ldots, r$,
  (b) $\mathrm{conv}(C_j) \cap \mathrm{conv}(C_k)$ is a common face of $\mathrm{conv}(C_j)$ *and* of $\mathrm{conv}(C_k)$ for all pairs $C_j, C_k \in \mathcal{S}$,
  (c) $\bigcup_{j=1}^{r} \mathrm{conv}(C_j) = \mathrm{conv}(\mathcal{A})$.

(ii) The subdivision is called *mixed* if the additional property

  (d) $\sum_{\lambda=1}^{l+2} \dim(\mathrm{conv}(C_j^{(\lambda)})) = m$ for all cells $C_j \in \mathcal{S}$ holds.

(iii) A cell C_j is called *mixed*, if

  (e) $\dim(\mathrm{conv}(C_j^{(\lambda)})) = k_\lambda, \quad \lambda = 1, \ldots, l+2.$

(iv) A mixed cell C_j is called *simple*, if

  (f) $\sum_{\lambda=1}^{l+2} (\#(C_j^{(\lambda)}) - 1) = m$ holds.

(v) A mixed subdivision is called a *simple mixed* subdivision if all mixed cells are simple mixed cells.

The definition of mixed subdivision is important since $\sum_j \mathrm{vol}(C_j)$ is the number of complex solutions in $(\mathbf{C} \setminus \{0\})^m$ for generic coefficients (Theorem by Bernstein, see Cox *et al.*, 1998). The proof in Huber and Sturmfels (1995) gives some insight into the number of real solutions. But first we need another definition.

DEFINITION. A simple mixed cell C is called *alternating* if the associated small initial system

$$\sum_{y \in C^{(\lambda)}} c_{ij} x^y = 0, \qquad \lambda = 1, \ldots, l+2, \qquad i = 1, \ldots, k_\lambda,$$

has exactly one positive solution.

This definition was introduced in Itenberg and Roy (1996) and Sturmfels (1998) in the case where each equation has different support and the associated small initial systems consist of binomials. By the Smith normal form it is known that binomial systems have one real solution if and only if the signs of the coefficients are alternating in each binomial equation.

The number of positive solutions of $\mathcal{H}(\varepsilon, x)$ for ε small equals the number of alternating cells. If nothing goes wrong along the homotopy (see Figure 6) then the number of alternating cells gives the number of positive solutions of system (5).

THEOREM 8.1. (STURMFELS, 1998) *Consider* $YA\Psi(x) = 0, v_i^t x - a_i = 0, i = 1, \ldots,$ rank (YA) *with fixed values of the parameters* k_{ij} *and* a_i. *There is a polynomial* $P(t) \in \mathbf{R}[t]$ *with the following property: if* $P(t)$ *has no solution in* $(0, 1]$ *and the initial systems associated to the facets* F *of the Newton polytopes do not have infinitely many solutions for some* $t \in (0, 1]$ *then the number of positive solutions of* $YA\Psi(x) = 0$ *in* $\{x \in (\mathbf{R}_+)^m \mid v_i^t x - a_i = 0, i = 1, \ldots, m - \operatorname{rank}(YA)\}$ *equals the number of alternating cells in a simple mixed subdivision.*

The theoretical background may be found in Sturmfels (1994a, 1998).

REMARK. (i) The polynomial $P(t) \in \mathbf{R}[c_{ij}, b_{ij}, a_i][t]$ is the sparse resultant $Res_{\mathcal{B}}(t; k, a)$ in $\mathbf{R}[k_{ij}, a_i][t]$ where $\mathcal{B}$ is given by the supports $\mathcal{A}_1, \ldots, \mathcal{A}_{l+2}$ and the support of the determinant of the toric Jacobian. (ii) The second assumption on infinitely many solutions of the small initial system associated to a facet is the condition from toric geometry that the original system has a solution at infinity or with zero components. Here it guarantees that no real negative solution turns positive (or from positive to negative) along the path.

EXAMPLE 8.2. We illustrate Theorem 8.1 with the example by Edelstein (Feinberg, 1979, pp. 2–26) with three variables, five complexes and two connected components, see Figure 7.

$$Y = \begin{bmatrix} 1 & 2 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \quad A = \begin{bmatrix} -k_{2,1} & k_{1,2} & 0 & 0 & 0 \\ k_{2,1} & -k_{1,2} & 0 & 0 & 0 \\ 0 & 0 & -k_{4,3} & k_{3,4} & 0 \\ 0 & 0 & k_{4,3} & -k_{3,4} - k_{5,4} & k_{4,5} \\ 0 & 0 & 0 & k_{5,4} & -k_{4,5} \end{bmatrix},$$

are the matrices given by the bipartite graph and the directed graph, respectively. The

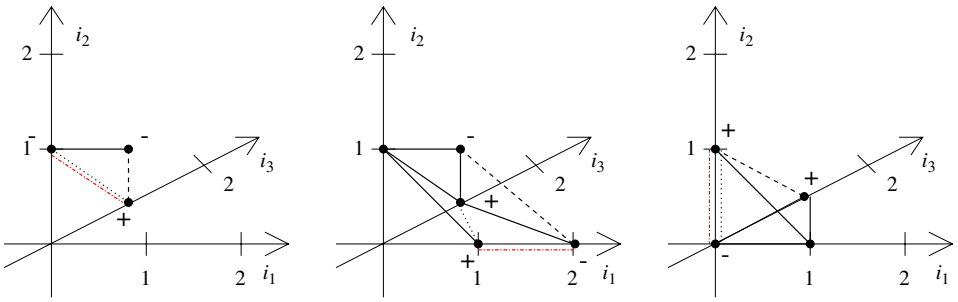

Figure 9. Mixed subdivision of Newton polytopes of the system by Edelstein. One of the three mixed cells is alternating.

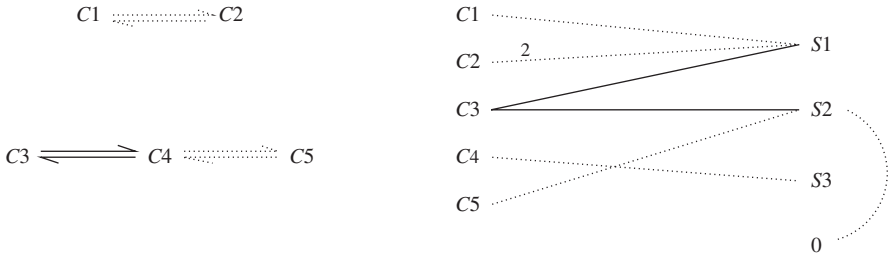

Figure 10. Parts of the directed graph of the example by Edelstein which corresponds to the alternating cell which is responsible for the positive solution.

differential equations are

$$\begin{aligned}
\dot{x}_1 &= k_{2,1}x_1 - k_{1,2}{x_1}^2 - k_{4,3}x_1x_2 + k_{3,4}x_3,\\
\dot{x}_2 &= -k_{4,3}x_1x_2 + (k_{3,4} + k_{5,4})\,x_3 - k_{4,5}x_2,\\
\dot{x}_3 &= k_{4,3}x_1x_2 + (-k_{3,4} - k_{5,4})\,x_3 + k_{4,5}x_2.
\end{aligned}$$

The polynomial system $\dot{x} = 0$ on a subspace is equivalent to

$$\begin{aligned}
0 &= -k_{4,3}x_1x_2 + (k_{3,4} + k_{5,4})\,x_3 - k_{4,5}x_2, && (\lambda = 2, i = 1)\\
0 &= k_{2,1}x_1 - k_{1,2}{x_1}^2 - k_{4,3}x_1x_2 + k_{3,4}x_3 + 0 \cdot x_2, && (\lambda = l+1 = 3, i = 1)\\
0 &= 0 \cdot x_1 + x_2 + x_3 - a, && (\lambda = l+2 = 4, i = 1)
\end{aligned}$$

with $v_1 = (0, 1, 1)$. For positive a the set $\{x \in (\mathbf{R}_+)^3 \,|\, v_1^t x - a = 0\}$ is non-empty. Figure 8 shows the Newton polytopes. Since there are two coefficients zero one may consider even sparser Newton polytopes. We do not do this here and concentrate on the general structure. The lifting

$$\begin{aligned}
\widehat{\mathcal{A}_1} = \{\},\quad \widehat{\mathcal{A}_2} &= \{(1,1,0,8),(0,0,1,0),(0,1,0,2)\},\\
\widehat{\mathcal{A}_3} &= \{(1,0,0,0),(2,0,0,5),(1,1,0,4),(0,0,1,0),(0,1,0,9)\},\\
\widehat{\mathcal{A}_4} &= \{(0,0,0,5),(1,0,0,20),(0,1,0,0),(0,0,1,-1)\},
\end{aligned}$$

gives a mixed subdivision with three simple mixed cells

$$C^{(2)} = \{\hat{y}_3, \hat{y}_4\},\ C^{(3)} = \{\hat{y}_2, \hat{y}_3\},\ C^{(4)} = \{\hat{e}_2, \hat{e}_3\}, \qquad \gamma = (-7, -6, -5, 1),$$
$$C^{(2)} = \{\hat{y}_4, \hat{y}_5\},\ C^{(3)} = \{\hat{y}_1, \hat{y}_2\},\ C^{(4)} = \{\hat{e}_1, \hat{e}_3\}, \qquad \gamma = (7, 5, -5, 1),$$
$$C^{(2)} = \{\hat{y}_4, \hat{y}_5\},\ C^{(3)} = \{\hat{y}_1, \hat{y}_4\},\ C^{(4)} = \{\hat{e}_1, \hat{e}_2\}, \qquad \gamma = (5, 7, 7, 1),$$

as shown in Figure 9. Obviously, there is one alternating cell for $a > 0$ and none for $a < 0$. So we expect for some region of the parameters k_{ij} one positive solution within a space $\{x \in (\mathbf{R}_+)^3 \mid v_1^t x - a = 0\} = (\frac{a}{2} v_1 + \mathrm{im}(YA)) \cap (\mathbf{R}_+)^3$. The alternating cell is part of the Newton polytopes which in turn are given by the directed graph and the bipartite graph. Figure 10 shows the parts of the graphs which correspond to the alternating cell and thus to the positive solution. There might be the chance for a subdivision with three cells as well. This example has from one to three positive solutions.

The condition in Theorem 8.1 tells us that we have to expect as many real positive solutions as there are alternating cells in the subdivision if the coefficients of the alternating cells are dominant against the rest of the coefficients. In this context of chemical reaction systems the coefficients are of very different magnitude since the rate constant of a forward reaction is very different from the rate constant of the associated backward reaction. We conclude that for chemical reaction systems Theorem 8.1 gives a realistic estimate for the number of positive solutions. The alternating cells as parts of the Newton polytopes correspond to parts of the directed graph. We conclude that we can identify parts of the directed graph which are responsible for positive solutions for some parameter region.

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