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A family of sparse polynomial systems arising in chemical reaction systems

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A family of sparse polynomial systems arising in chemical reaction systems

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Abstract: A class of sparse polynomial systems is investigated which is defined by a weighted directed graph and a weighted bipartite graph. They arise in the model of mass action kinetics for chemical reaction systems. In this application the number of real positive solutions within a certain affine subspace is of particular interest. We show that the simplest cases are equivalent to binomial systems while in general the solution structure is highly determined by the properties of the two graphs. First we recall results by Feinberg and give rigorous proofs. Secondly, we explain how the graphs determine the Newton polytopes of the system of sparse polynomials and thus determine the solution structure. The 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 arise in applications. These systems arise in the modelling 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.

In the chemical engineering literature [3, 8, 9, 10, 11, 14, 16, 23] there have been several attempts to study the number of real positive solutions depending on the structure of the graphs.

The investigation of real positive solutions of the sparse polynomial system $f(x) = 0$ is very important for the application since this are the steady state solutions of a dynamical system $\dot{x} = f(x)$ which in turn is just 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 of a monomial influences the existence of time- and space-dependent solutions of the reaction diffusion system. Secondly, singular perturbation theory of $\dot{x} = f(x)$ exploits the knowledge of the real variety for the investigation of properties of periodic

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orbits. The decomposition into slow and fast variables is done in cases where a periodic orbit is close to the real variety. Dynamic phenomena of systems of mass action type have been studied a lot by numerical mathematicians, see e.g. [6].

The studies by engineers are 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 [21] Gröbner basis computation for systems of mass action type have been performed. We do not follow this approach. The homotopy method [18] 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 e.g. [19, 30, 31]. Other homotopy methods are suggested in [17].

Related to this approach there are results on the number of real and of positive real solutions [20, 27, 28]. In [29] Sturmfels gives an easy to read summary of these approaches. In the last section we apply these results to our particular application.

The aim of this paper is to build a bridge between the two areas, the chemical engineering literature and the algebraic literature on sparse polynomial systems. We give a mathematical introduction into the model and rigorous proofs of the results in the engineering literature. The application of the results of sparse polynomial systems gives a deeper understanding and transparence. Our main result is that cycles and paths in the directed graph are closely related to the existence of positive solutions.

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 kinetic matrix A this is investigated in Section 3. In Sections 4, 5, and 6 the simple cases with $\operatorname{rank}(A) = \operatorname{rank}(YA)$ or $\operatorname{rank}(A) = \operatorname{rank}(YA)+1$ are treated. The previous results by Feinberg[1] are proved rigorously. The binomial systems are solved with Smith normal form or Hermite normal form while the dimension of the generated lattice and toric varieties are exploited in other cases.

Finally, the last section applies the theory of sparse polynomial systems.
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.

The data are 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 *complexes* C_i. Each oriented edge $C_j \to C_i$ has a weight $k_{C_j \to C_i} = k_{ij} \in \mathbf{R}_+$. This defines the weighted adjacency matrix $K = (k_{ij}) \in (\mathbf{R}_{\geq 0})^{n,n}$ with $k_{ij} = 0$ if $C_j \to C_i$ is not an arrow. The second graph

[1] Feinberg writes in [11]: Charlie Conley was very enthusiastic about chemical reaction network theory, and, for me, his enthusiasm was a source of encouragement when encouragement was very much needed. At the time, I did not know that Charlie was enthusiastic about everything.

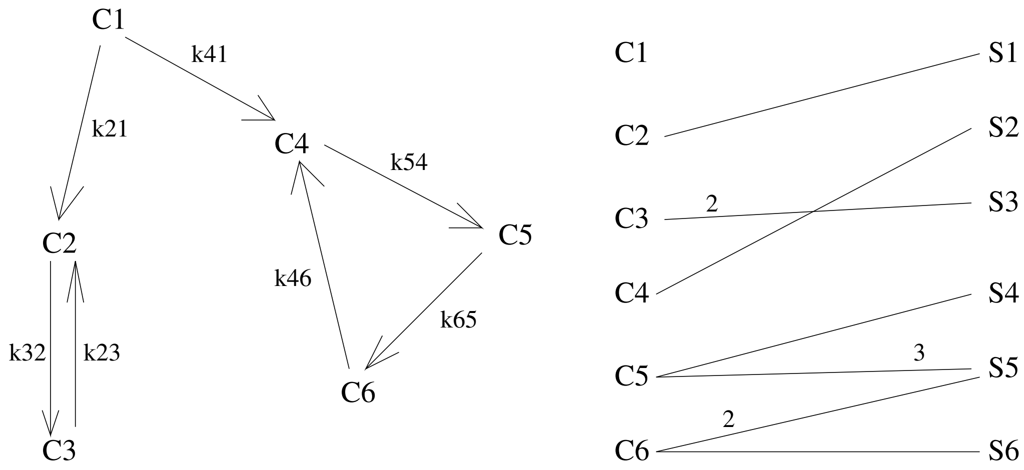

Figure 1: A reaction network with six complexes as a weighted directed graph and a weighted bipartite graph for the composition of complexes as sums of species.

is a *weighted bipartite graph* encoding the occurence of species in the complexes. The two sets consists of the chemical *species* S_i, $i = 1, \ldots, m$ and the complexes C_j, $j = 1, \ldots, n$. Each edge $\{C_j\, S_i\}$ has a weight $y_{ij} \in \mathbf{N}$. This defines the weighted adjacency matrix whose relevat part is $Y = (y_{ij})_{i=1,\ldots,m, j=1,\ldots,n}$. It is called *stoichiometric matrix* since the complexes are given as $C_j = \sum_{i=1}^m y_{ij} S_i$, $j = 1, \ldots, n$ with *stoichiometric coefficients* y_{ij}. We call the columns of Y by $y_1, \ldots, y_n \in (\mathbf{Z}_{\geq 0})^m$.

There are some restrictions on the directed graph R in order to be non-degenerate. For example each C_i appears at least once on the left or the right of an oriented edge. But 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 complexes only appear as results and thus are called *product complexes.* The number of the *reactant complexes* is denoted by r. Obviously, $r \leq n$. In the bipartite graph it may happen that one complex C_j is not linked to the species S_i and thus the associated column is $y_j = 0$ since this corresponds to the fact that a chemical substance is constantly poured into the chemical reactor. But we assume that every vertex S_i is linked to a complex C_j.

The model of mass action kinetics is built from three mappings resulting in a system of differential equations consisting of sparse polynomials.
1.) The directed graph R defines a linear mapping A which encodes the information about the reaction probabilities. The amout of reaction $C_j \to C_i$ taking place depends on the presence of the species in C_j. This 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. So let the unit vectors of $\mathbf{R}^n$ denote by $\omega_1, \ldots, \omega_n$. Then

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

is a linear mapping measuring the changes. Since

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

the representing matrix of the mapping A with respect to the standard basis $\omega_1, \ldots, \omega_n$ of $\mathbf{C}^n$ is the *kinetic matrix* $A = (K - \mathrm{diag}(K^t e))$, where $e = (1, \ldots, 1)^t \in \mathbf{R}^n$. Observe that $n - r$ columns of A corresponding to product complexes are zero. Often we will restrict to the non-negative orthant $(\mathbf{R}_{\geq 0})^n$ or to the positive orthant $(\mathbf{R}_+)^n$ where $\mathbf{R}_+$ denotes the positive real numbers and $\mathbf{R}_{\geq 0}$ denotes the non-negative real numbers. The rank of the linear mapping A depends of course on the values of k_{ij}. But it strongly depends on the structure of the graph as the following example shows.

Example 2.1 *The network in Figure 1 contains $n = r = 6$ complexes. The mapping $A : \mathbf{C}^6 \to \mathbf{C}^6$ is given by*

$$\begin{aligned}
A(u) &= k_{21}u_1(\omega_2 - \omega_1) + k_{32}u_2(\omega_3 - \omega_2) + k_{23}u_3(\omega_2 - \omega_3) \\
&\quad + k_{41}u_1(\omega_4 - \omega_1) + k_{54}u_4(\omega_5 - \omega_4) + k_{65}u_5(\omega_6 - \omega_5) + k_{46}u_6(\omega_4 - \omega_6) \\
&= k_{21}u_1(\omega_2 - \omega_1) + (k_{32}u_2 - k_{23}u_3)(\omega_3 - \omega_2) + k_{41}u_1(\omega_4 - \omega_1) + \\
&\quad (k_{54}u_4 - k_{46}u_6)(\omega_5 - \omega_4) + (k_{65}u_5 - k_{46}u_6)(\omega_6 - \omega_5) \\
&= \begin{pmatrix} (-k_{21} - k_{41})u_1 \\ k_{21}u_1 - k_{32}u_2 + k_{23}u_3 \\ k_{32}u_2 - k_{23}u_3 \\ k_{41}u_1 - k_{54}u_4 + k_{46}u_6 \\ k_{54}u_4 - k_{65}u_5 \\ k_{65}u_5 - k_{46}u_6 \end{pmatrix} \\
&= \begin{pmatrix} -(k_{21} + k_{41}) & & & & & \\ k_{21} & -k_{32} & +k_{23} & & & \\ & k_{32} & -k_{23} & & & \\ k_{41} & & & -k_{54} & & k_{46} \\ & & & k_{54} & -k_{65} & \\ & & & & k_{65} & -k_{46} \end{pmatrix} u.
\end{aligned}$$

The rank of the matrix is 4 for generic choice of k_{ij} since $(0,1,1,0,0,0)A = 0$ and $(0,0,0,1,1,1)A = 0$. In Section 3 it will be explained that this is due to the special structure of the directed graph.

2.) For each complex there is a monomial in the variables $x_1, \ldots, x_m$ which are the concentrations of the species. Then

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

comes in whenever something depends on the concentrations x of the species.

Since concentrations are non-negative one often restricts Ψ to $(\mathbf{R}_+)^m$ or $(\mathbf{R}_{\geq 0})^m$. Obviously, $\mathrm{im}(\Psi_{|(\mathbf{R}_{\geq 0})^m}) \subset (\mathbf{R}_{\geq 0})^n$ and $\mathrm{im}(\Psi_{|(\mathbf{R}_+)^m}) \subset (\mathbf{R}_+)^n$.

3.) The third mapping is the linear mapping

$$Y : \mathbf{C}^n \to \mathbf{C}^m, \quad z \to \sum_{i=1}^{n} y_i z_i \,,$$

associated to the relevant part $Y = (y_1, \ldots, y_n) \in (\mathbf{Z}_{\geq 0})^{m,n}$ of the weighted adjacency matrix of the bipartite graph. $z_i = (Au)_i$ means the change of the i-th complex. The chemical substance S_j appears in some of these complexes with quantity $(y_j)_i = y_{ij}$. Thus $(Yz)_j$ gives the change of species S_j according to the changes of the complexes. The composition is

$$YA(u) = \sum_{(y_j \to y_i) \in R} k_{ij} u_j (y_i - y_j) \,.$$

Altogether we get 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.

Example 2.2 *(Example 2.1 continued). From Figure 1 we read from the bipartite graph the stoichiometric matrix*

$$Y = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 3 & 2 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

This gives the following differential equations

$$\begin{aligned}
\dot{x}_1 &= k_{2,1} - k_{3,2} x_1 + k_{2,3} {x_3}^2, \\
\dot{x}_2 &= k_{4,1} - k_{5,4} x_2 + k_{4,6} {x_5}^2 x_6, \\
\dot{x}_3 &= 2\, k_{3,2} x_1 - 2\, k_{2,3} {x_3}^2, \\
\dot{x}_4 &= k_{5,4} x_2 - k_{6,5} x_4 {x_5}^3, \\
\dot{x}_5 &= 3\, k_{5,4} x_2 - k_{6,5} x_4 {x_5}^3 - 2\, k_{4,6} {x_5}^2 x_6, \\
\dot{x}_6 &= k_{6,5} x_4 {x_5}^3 - k_{4,6} {x_5}^2 x_6
\end{aligned}$$

Problem: For a given directed graph R with non-negative constant weights $k_{ij} \in \mathbf{R}_{\geq 0}$, $i, j = 1, \ldots, n$ and complexes $y_i \in (\mathbf{Z}_{\geq 0})^m, i = 1, \ldots, n$ we have the sparse polynomial equations

$$YA\Psi(x) = \sum_{(C_j \to C_i) \in R} k_{ij} x^{y_j} (y_i - y_j) = 0 \,. \tag{2}$$

The task is to discuss the structure of the solutions in $(\mathbf{R}_+)^m$ and $(\mathbf{R}_{\geq 0})^m$.

Due to the structure arising from chemical reactions the systems often will be underdetermined. Thus one is allowed to add additional linear restrictions and still gets a solvable system. A natural choice are the affine linear subspaces $x_0 + \mathrm{im}(YA)$ since they are flow-invariant by the following lemma.

Lemma 2.3 *A trajectory $x : \mathbf{R} \to \mathbf{R}^m$ of the differential equations*

$$\dot{x} = YA\Psi(x)$$

starting at $x(t_0) = x_0 \in (\mathbf{R}_{\geq 0})^m$ for $t = t_0$ stays for all $t > t_0$ within the affine space $x_0 + im(YA)$. If the trajectory $x(t)$ stays within $(\mathbf{R}_{\geq 0})^m$ for all $t \in [t_0, t_1]$ then it stays in the cone $x_0 + \{\sum_j \alpha_j Y a_j \,|\, \alpha_j \geq 0, j = 1, \dots, n\}$ *where a_j denote the columns of A.*

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 the image of YA. Simple integration along the solution $x(t)$ yields

$$x(t_2) = x(t_1) + \int_{t_1}^{t_2} YA\Psi(x(t))dt.$$

This is equivalent to

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

which shows that the difference $x(t_2) - x(t_1)$ is a linear combination of the columns of YA with coefficients $\alpha_j = \int_{t_1}^{t_2} \Psi_j(x(t))dt = \int_{t_1}^{t_2} x^{y_j}(t)dt$.

If $x(t)$ is non-negative then the monomials x^{y_j} are non-negative and so are the coefficients α_j. $\square$

A trajectory staying in $(\mathbf{R}_{\geq 0})^m$ and in the cone $x_0 + \sum_j \alpha_j Y a_j$ stays in particular in $(x_0 + \mathrm{im}(YA)) \cap (\mathbf{R}_{\geq 0})^m$. In [9] $\mathrm{im}(YA)$ is called *kinetic subspace*.

Since the columns of A are linear combinations of $\omega_i - \omega_j$ where $C_j \to C_i$ are elements of the directed graph R Feinberg [8] p. 2-15 defines the so-called *stoichiometric space*

$$S = \mathrm{span}(\{y_i - y_j \,|\, (C_j \to C_i) \in R\}).$$

In [8] the space S is a natural choice since more general models which are not given by polynomial functions are considered. 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. But it is clear that the variation is a variation of subvector spaces of the stoichiometric space S. In the engineering literature Lemma 2.3 is formulated with S instead of $\mathrm{im}(YA)$. Additionally, one finds conditions under which $(x_0 + S) \cap (\mathbf{R}_{\geq 0})^m$ is a bounded region. Observe that S is related to the *incidence matrix* $W = (w_{\mu k}) \in \{-1, 0, 1\}^{n,a}$ of the directed graph with

$$w_{\mu k} = \begin{cases} 1 & \mu = i, \\ -1 & \mu = j, \\ 0 & \text{else} \end{cases}$$

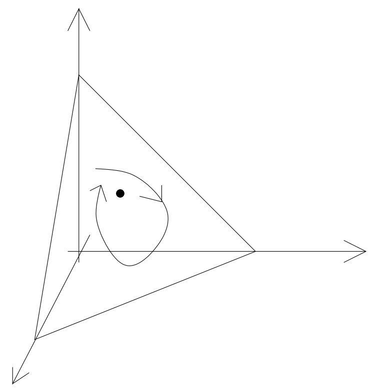

Figure 2: A trajectory within an affine subspace.

where $C_j \to C_i$ is the oriented edge (arrow) of index k and a is the number of arrows. Then $S = \mathrm{im}(YW)$.

It should be understood that the weighted directed graph and the weighted bipartite graph are often the result of modifications of the original chemical reaction system.

- The edge $0 \to S_i$ modells 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 where each chemical species given into the reactor immediately reacts to something else.

- Several oriented edges are often summarized as one edge by experience by insight into the chemical process by chemical engineers. In the elementary reactions the complexes consists most of the time of two species only.

- Often the model of mass action kinetics is modified by taking more general functions into account.

- A special modelling of the graphs is necessary for catalytic surface reactions where the chemical reaction only happens on the surface of a catalyst.

The main properties of the system of sparse polynomial equations are summarized as follows.

- The coefficients of the system are determined by the sparse structure of the directed graph by the mapping A and by the bipartite graph by its stoichiometric matrix Y.

- The coeficients y_{ij} of the complexes enter twice, as exponents in the monomials and in the coefficients.

- The system is a sparse system, but moreover sparse monomials appear only since the y_i have sparse support.

- Last not least the signs of the coefficients are (partially) restricted since $k_{ij} \geq 0$ and $(y_i)_l \geq 0$.

There are two tasks: studying the coefficient matrix and secondly to study the lattice generated by the exponents of the monomials. Since the coefficient matrix YA determines how the monomials are distributed over the polynomials both tasks are closely related. The first distinction is made whether the property $\operatorname{rank}(Ya) = \operatorname{rank}(A)$ is satisfied.
Obviously, one first needs to investigate the non-genericity of the coefficients. This is simply linear algebra. One has to distinguish the two cases
a.) $\operatorname{Rank}(Y_{|\operatorname{im}(A)}) = \operatorname{Rank}(A)$ or
b.) $\operatorname{Rank}(Y_{|\operatorname{im}(A)}) < \operatorname{Rank}(A)$.
In the engineering literature [8, 14] either case a.) is assumed where solving $YA\Psi(x) = 0$ is equivalent to solving $A\Psi(x) = 0$ or other conditions hold which imply case b.). In many situations these assumptions are well justified by the application.

3 The structure of the kinetic matrix A

Since the kinetic 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 multigraph. A standard notion of a graph is that of its *connected components* which are called in the engineering literature *linkage classes*. We refer to them as $\mathcal{L}_\lambda \subset \{1, \ldots, n\}, \lambda = 1, \ldots, l$ collecting the indices of connected vertices. Thus $\{1, \ldots, n\} = \mathcal{L}_1 \dot\cup \mathcal{L}_2 \dot\cup \cdots \dot\cup \mathcal{L}_l$. Since the graph R is directed the connected components may be even further decomposed.

Definition 3.1 *([8] p. 4-7) Two complexes C_i, C_j are called* strongly linked*, if a sequence of complexes exists such that $C_i \to C_{\nu_1} \to C_{\nu_2} \to \cdots \to C_j$ and a path exists with $C_j \to C_{\mu_1} \to C_{\mu_2} \to \cdots \to C_i$. This equivalence relations decomposes the set of complexes into the* strong connected components *or* strong linkage classes*. If no complex in a strong linkage class reacts to a complex not in this class, this class is called* terminal strong linkage class *or* terminal strong connected component*. We denote these terminal classes by $\mathcal{T}_\nu^\lambda \subset \{1, \ldots, r\}, \nu = 1, \ldots, t_\lambda$ where $t_1 + \cdots + t_l = t$ is their total number.*

These definitions are illustrated in the following example. It shows the consequences for their structure of the mapping A.

Example 3.2 *The chemical reaction in Figure 3 includes $n = r = 12$ complexes.*

There are three connected components $\mathcal{L}_1 = \{1, 2, 3\}, \mathcal{L}_2 = \{4, 5, 6, 7, 8, 9\}, \mathcal{L}_3 = \{10, 11, 12\}$. The first class $\mathcal{L}_1$ includes the strong linkage class $\{1, 2\}$ and the terminal strong linkage class $\mathcal{T}_1^1 = \{3\}$ while the second class subdivides into two terminal strong linkage classes, $\mathcal{T}_1^2 = \{5, 6, 7\}, \mathcal{T}_2^2 = \{8, 9\}$ and one strong linkage class equal to $\{4\}$. The fourth terminal strong linkage class is $\mathcal{T}_1^3 = \mathcal{L}_3$. The rests $\mathcal{R}_1 = \mathcal{L}_1 \setminus \mathcal{T}_1^1 = \{1, 2\}$ and

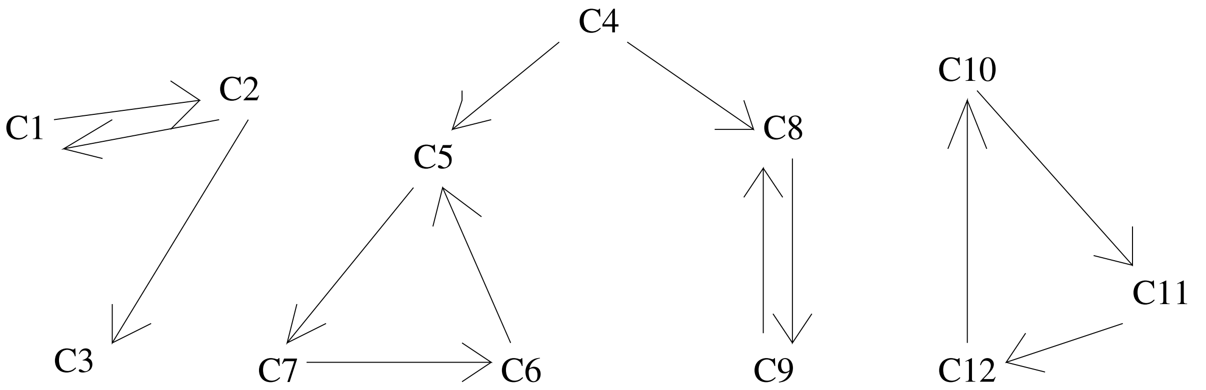

Figure 3: A reaction network with three connected components (linkage classes), four terminal strong linkage classes and two strong linkage classes which are not terminal.

$\mathcal{R}_2 = \mathcal{L}_2 \setminus (\mathcal{T}_1^2 \cup \mathcal{T}_2^2) = \{4\}$ *are strong linkage classes. In general the rest (connected component minus terminal strong linkage classes) may decompose into several strong linkage classes.*

It is worth to look at the kinetic matrix A since it has a particular structure.

$$A = \begin{pmatrix} A_1 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & A_3 \end{pmatrix} \quad \textit{with} \quad A_1 = \left(\begin{array}{rr|r} -k_{21} & k_{12} & 0 \\ k_{21} & -k_{12} - k_{32} & 0 \\ \hline 0 & k_{32} & 0 \end{array}\right) \quad \textit{and}$$

$$A_2 = \left(\begin{array}{r|rrr|rr} -k_{54} - k_{84} & 0 & 0 & 0 & 0 & 0 \\ \hline k_{54} & -k_{65} & 0 & k_{57} & 0 & 0 \\ 0 & k_{65} & -k_{76} & 0 & 0 & 0 \\ 0 & 0 & k_{76} & -k_{57} & 0 & 0 \\ \hline k_{84} & 0 & 0 & 0 & -k_{98} & k_{89} \\ 0 & 0 & 0 & 0 & k_{98} & -k_{89} \end{array}\right), \quad A_3 = \begin{pmatrix} -k_{11,10} & 0 & k_{12,10} \\ k_{11,10} & -k_{12,11} & 0 \\ 0 & k_{12,11} & -k_{12,10} \end{pmatrix}.$$

Each connected component corresponds to an invariant subspace of A which further decomposes into invariant subspaces corresponding to terminal strong linkage classes and a non-invariant rest. Observe that the four submatrices corresponding to the terminal strong linkage classes have rank defect one each.

Lemma 3.3 *The vector space $\mathbf{C}^n$ decomposes into vector spaces according to the connected components which are invariant under A, i.e. $\exists\, L_\lambda = span(\{\omega_\lambda \,|\, \mu \in \mathcal{L}_\lambda\})$ with*

$$\mathbf{C}^n = L_1 \oplus \cdots \oplus L_l \quad \textit{and} \quad AL_\lambda \subset L_\lambda, \;\; \lambda = 1, \ldots, l.$$

Each L_λ further decomposes according to the terminal strong linkage classes, i.e. for each $\lambda = 1, \ldots, l$ one defines $T_\nu^\lambda := span(\{\omega_i \,|\, i \in \mathcal{T}_\nu^\lambda\})$ for $\nu = 1, \ldots, t_\lambda$ and the rest $R_\lambda := span(\{\omega_i \,|\, i \in \mathcal{R}_\lambda = \mathcal{L}_\lambda \setminus \bigcup_{\nu=1}^{t_\lambda} \mathcal{T}_\nu^\lambda\})$. Then for all $\lambda = 1, \ldots, l$

$$L_\lambda = T_1^\lambda \oplus \cdots \oplus T_{t_\lambda}^\lambda \oplus R_\lambda \quad \textit{with} \quad AT_\nu^\lambda \subset T_\nu^\lambda, \;\; \nu = 1, \ldots, t_\lambda\,.$$

Especially, each pure product complex forms one terminal strong linkage class. 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_ν^λ =span(ω_i).

Theorem 3.4 *([14], Prop. 4.1 in [8]) The kernel of the kinetic mapping A decomposes as*

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

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

$$\begin{aligned} (v_\nu^\lambda)_i &> 0 \quad \text{for } i \in \mathcal{T}_\nu^\lambda, \\ (v_\nu^\lambda)_i &= 0 \quad \text{for } i \in \{1, \ldots, n\} \setminus \mathcal{T}_\nu^\lambda. \end{aligned}$$

Remark 3.5 *This theorem is heavily based on the fact that the rate constants k_{ij} associated to an oriented edge in the directed graph R are positive.*

For convenience we recall the proof in the Appendix.

Decomposing the kinetic matrix A according to the connected components and terminal strong linkage classes by

$$A = \begin{pmatrix} A_1 & & \\ & \ddots & \\ & & A_l \end{pmatrix}, \quad A_\lambda = \begin{pmatrix} B & 0 & \cdots & 0 \\ B_1 & A_{\lambda 1} & & 0 \\ \vdots & & \ddots & \\ B_{t_\lambda} & 0 & & A_{\lambda t_\lambda} \end{pmatrix}, \quad \lambda = 1, \ldots, l,$$

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 linkage classes within the connected component λ. Thus $\text{rank}(A) = n - t$ where t is the total number of terminal strong linkage classes.

The following defines a case with the most simplest structure of A.

Definition 3.6 *([8]) The directed graph R is called* weakly reversible*, if for each path $C_j \to C_{\nu_1} \to C_{\nu_2} \to \cdots \to C_i$ there is a path $C_i \to C_{\mu_1} \to C_{\mu_2} \to \cdots \to C_j$.*

In a weakly reversible graph each connected component equals its terminal strong linkage class. Chemists report that almost all relevant chemical reaction systems have this property. For weakly reversible graphs we have $\text{rank}(A) = n - l$ where l is the number of connected components. But $\text{rank}(A) = n - l$ may be true for graphs which are not weakly reversible. It is sufficient that each connected component contains precisely one terminal strong linkage class ($t_\lambda = 1$, $\lambda = 1, \ldots, l$).

Now we return to the coefficient matrix YA of our sparse polynomial system. $\text{im}(YA)$ equals $\text{span}(Ya_1, \ldots, Ya_n)$ where the a_j are the columns of A. On the other hand each a_j is a vector in $W = \text{span}(\omega_i - \omega_j \,|\, C_j \to C_i \in R)$, the image of the incidence matrix of the directed graph. If the graph is weakly reversible then $\mathrm{im}(A) = W$. The relation of the stoichiometric space $S = YW = \mathrm{span}(y_i - y_j \,|\, C_j \to C_i \in R)$ to W is analogous to the relation of $\mathrm{im}(YA)$ to $\mathrm{span}(a_1, \ldots, a_n) = \mathrm{im}(A)$. Since $\mathrm{im}(A) \subseteq W$ it follows $\mathrm{im}(YA) \subseteq S$. If $\dim(S) = \dim(W)$ then $\dim(\mathrm{im}(YA)) = \dim(\mathrm{im}(A))$ by the same argumentation. Secondly,

$$\dim(W) - \dim(S) \geq \dim(\mathrm{im}(A)) - \dim(\mathrm{im}(YA)).$$

Feinberg [8] shows that $\dim(W) = n - l$ where l is the number of connected components. Then he calls $\delta = \dim(W) - \dim(S) = n - l - \dim(S)$ the *deficiency*. It is simply the rank defect between W and $YW = S$. But we need to know the rank defect between $\mathrm{im}(A)$ and $\mathrm{im}(YA)$. If the graph is weakly reversible then $\mathrm{im}(YA) = S$ and the deficiency measures the correct rank defect. Analogously, if each connected component contains precisely one terminal strong linkage class only then $\mathrm{im}(A) = W$ implies $\mathrm{im}(YA) = S$ and the deficiency is useful.

4 A first result

We give results for a special class of chemical reaction systems of mass action type. The first is our version of the deficiency zero theorem ([9]). The theorem uses the Smith normal form which may be found in the text books [1] p. 307 and [22] Section 1.4. For efficient computations of Smith normal forms for sparse integer matrices see [24]. For practical computations one often uses the Hermite normal form, see [1] p. 301. For its efficient implementation see [25, 26].

Theorem 4.1 *Consider the system $YA\Psi(x) = 0$ with $A = K - diag(K^t e)$ with $e = (1, \ldots, 1)$ defined by the weighted adjacency matrix K of a directed graph and the relevant part Y of an adjacency matrix of a weighted bipartite graph. If the directed graph is weakly reversible and*

$$rank(A) = rank(YA),$$

then each space $(x_0 + im(YA)) \cap (\mathbf{R}_+)^m$ with $x_0 \in (\mathbf{R}_+)^m$ contains precisely one real positive solution of $YA\Psi(x) = 0$.

Proof: Since $rank(A) = \mathrm{rank}(YA)$ solving $YA\Psi(x) = 0$ is equivalent to solving $A\Psi(x) = 0$. Since the directed graph is weakly reversible the kinetic matrix A has block diagonal form where each block has rank defect 1. Since the graph is weakly reversible $\mathrm{im}(YA)$ equals the stoichiometric space S. Its dimension is $\mathrm{rank}(YA) = \mathrm{rank}(A) = \dim(S)$ and we denote it by s. By linear algebra and Theorem 3.4 the system $A\Psi(X) = 0$ is equivalent to solving a system of s binomial equations

$$x^{y_i} - c_1 x^{y_j} = 0, \quad \ldots \quad , x^{y_k} - c_s x^{y_l} = 0.$$

In each equation the exponents of the two binomials correspond to two complexes in the same connected component. Moreover, the constants $c_1, \ldots, c_s$ are positive since the diagonal elements of A are negative dominant ($a_{jj} \leq -\sum_{i \neq j} a_{ij}, j = 1, \ldots, n$). This property is preserved under Gaussian elimination. Since only positive solutions are interesting we may divide by one monomial

$$x^{y_i - y_j} = c_1, \quad \ldots \quad , x^{y_k - y_l} = c_s.$$

we receive exponents which generate the stoichiometric space S. Systems of binomial type may be solved by Smith normal form. The exponent vectors $y_i - y_j$ form the columns of a matrix $\Pi \in \mathbf{Z}^{m,s}$. There exists invertible integer matrices $U \in GL(m, \mathbf{Z}), V \in GL(s, \mathbf{Z})$ and $d_1, \ldots, d_s \in \mathbf{N}$ with $d_j | d_{j+1}, j = 1, \ldots, s-1$ such that

$$U \, \Pi \, V = \begin{pmatrix} d_1 & & 0 \\ & \vdots & \\ 0 & & d_s \\ & \mathbf{0} & \end{pmatrix}.$$

All invariant factors d_j are unequal zero since $\mathrm{span}(\Pi) = S$. The nonlinear change of coordinates

$$x_1 = z_1^{u_{11}} z_2^{u_{21}} \cdots z_m^{u_{m1}}, \quad \ldots, \quad x_m = z_1^{u_{1m}} z_2^{u_{2m}} \cdots z_m^{u_{mm}},$$

and exponentiation with entries of V and multiplication of equations yields

$$z_1^{d_1} = c_1', \quad \ldots \quad , z_s^{d_s} = c_s',$$

with $c_i' = \prod_{j=1}^{s} c_j^{v_{ji}} > 0, i = 1, \ldots, s$. Since the constants c_i' are positive there is precisely one positive solution $(\tilde{z}_1, \ldots, \tilde{z}_s)$. Positive values z correspond to positive x. For $z_{s+1}, \ldots, z_m$ there is no restriction giving a parametrization $x(z_{s+1}, \ldots, z_m)$ of the solution variety. 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 i-th row of U which for $i = s+1, \ldots, m$ is orthogonal to $\mathrm{im}(YA) = S = \mathrm{span}(\Pi)$. If x is positive $\mathrm{diag}(1/x_1, \ldots, 1/x_m)$ defines a weighted inner product. With respect to this locally defined inner product $\frac{\partial x}{\partial z_i}$ is orthogonal to S. This shows that the real positive variety is always transversal to the affine spaces $x_0 + \mathrm{im}(YA)$.
$\square$

Remark: Let the graph R be weakly reversible so that $S = \mathrm{im}(YA)$ and assume $\mathrm{rank}(YA) = \mathrm{rank}(A)$. For positive solutions $x, \tilde{x} \in (\mathbf{R}_+)^m$ we have

$$\begin{aligned} \ln(x) - \ln(\tilde{x}) &= U^t(\ln(z) - \ln(\tilde{z})) = (U_1^t, U_2^t) \left(\begin{pmatrix} \ln(z_1) \\ \ln(z_2) \end{pmatrix} - \begin{pmatrix} \ln(z_1) \\ \ln(\tilde{z}_2) \end{pmatrix} \right) \\ &= U_2^t \left(\ln(z_2) - \ln(\tilde{z}_2) \right). \end{aligned}$$

Here the logarithm of a vector is meant to be taken for each component and the indices 1 and 2 refer to two blocks of components corresponding to free and fixed variables. The

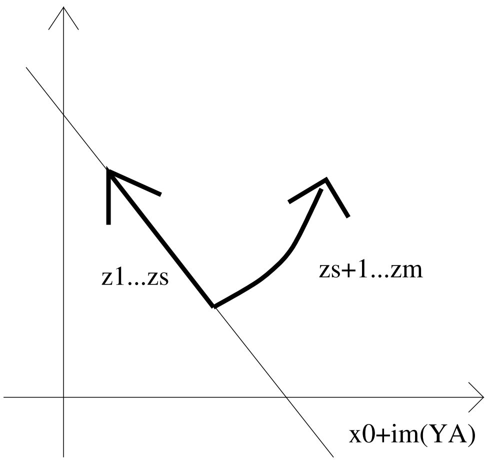

Figure 4: Nonlinear parametrization derived from Smith normal form.

last expression shows that the difference $\ln(x) - \ln(\tilde{x})$ is a linear combination of the last rows of U which in turn is a basis of $S^{\perp}$. In other words the free variables $z_{s+1}, \ldots, z_m$ give a nonlinear parametrization of $\mathrm{im}(YA)^{\perp}$. This agrees with the results in [8] p. 5-6 Prop. 5.3.

The technique using the logarithm in [8] is closely related to the techniques used in the algebraic geometry literature, especially [20] where the logarithm is used to solve a binomial system instead of using the Smith normal form as above.

Example 4.2 *(simple cycle) Consider the chemical reaction system in Figure 5. The matrix A is given by*

$$\begin{pmatrix} -k_{21} & 0 & 0 & k_{14} \\ k_{21} & -k_{32} - k_{42} & 0 & k_{24} \\ 0 & k_{32} & -k_{43} & 0 \\ 0 & k_{42} & k_{43} & -k_{14} - k_{24} \end{pmatrix}.$$

Assume YA has the same rank than A then we only need to consider $A\psi(x) = 0$ which is by Gaussian elimination equivalent to the binomial system

$$\begin{aligned} x^{y_1} \quad & -\tfrac{k_{1,4}}{k_{2,1}} \, x^{y_4} = 0\,, \\ x^{y_2} \quad & +\tfrac{k_{1,4}+k_{2,4}}{-k_{3,2}-k_{4,2}} \, x^{y_4} = 0\,, \\ x^{y_3} \quad & +\tfrac{(k_{1,4}+k_{2,4})k_{3,2}}{(-k_{3,2}-k_{4,2})k_{4,3}} \, x^{y_4} = 0\,. \end{aligned}$$

This is equivalent to

$$\begin{aligned} x^{y_1-y_4} &= \tfrac{k_{1,4}}{k_{2,1}}\,, \\ x^{y_2-y_4} &= \tfrac{k_{1,4}+k_{2,4}}{k_{3,2}+k_{4,2}}\,, \\ x^{y_3-y_4} &= \tfrac{(k_{1,4}+k_{2,4})k_{3,2}}{(k_{3,2}+k_{4,2})k_{4,3}}\,. \end{aligned}$$

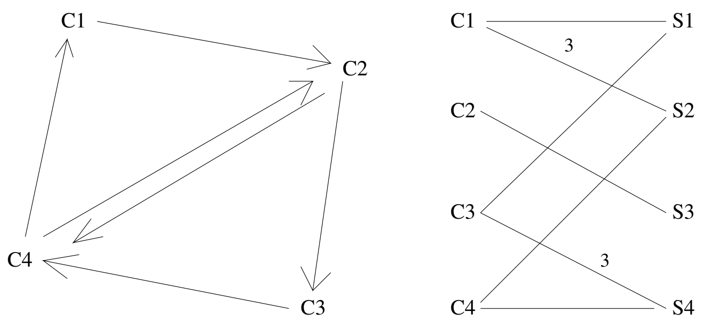

Figure 5: A Simple cycle with four complexes.

Choosing the bipartite graph as in Figure 5 with

$$y_1 = \begin{bmatrix} 1 \\ 3 \\ 0 \\ 0 \end{bmatrix}, \quad y_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \quad y_3 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 3 \end{bmatrix}, \quad y_4 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}$$

we have rank$(YA) =$*rank*$(A) = 3$. *Thus* $\Pi = (y_4 - y_1, y_2 - y_3, y_4 - y_2)$ *has maximal rank* 3 *and its Smith norm form is*

$$U\Pi V = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 2 & -1 & -1 & 0 \\ -1 & 1 & 2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 1 \\ 2 & -1 & -1 \\ 0 & 1 & 0 \\ -1 & -1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \\ 0 & 0 & 0 \end{bmatrix}.$$

Using the nonlinear change of coordinates $x_1 = z_1 z_3^2 z_4^{-1}$, $x_2 = z_3^{-1} z_4$, $x_3 = z_2 z_3^{-1} z_4^2$ *and* $x_4 = z_4$ *defined by* U *implies* $z_1 = \frac{k_{1,4}}{k_{2,1}}$, $z_2 = -\frac{k_{1,4}+k_{2,4}}{-k_{3,2}-k_{4,2}}$, $z_3 = \left(\frac{(k_{1,4}+k_{2,4})k_{3,2}k_{2,1}}{(k_{3,2}+k_{4,2})k_{4,3}k_{1,4}}\right)^{\frac{1}{3}}$ *and thus the solution*

$$\begin{aligned} x_1 &= {z_4}^{-1} \frac{k_{1,4}}{k_{2,1}} \left(\frac{(k_{1,4}+k_{2,4})k_{3,2}k_{2,1}}{(k_{3,2}+k_{4,2})k_{4,3}k_{1,4}}\right)^{\frac{2}{3}} \\ x_2 &= z_4 \left(\frac{(k_{1,4}+k_{2,4})k_{3,2}k_{2,1}}{(k_{3,2}+k_{4,2})k_{4,3}k_{1,4}}\right)^{-\frac{1}{3}} \\ x_3 &= {z_4}^2 \frac{(k_{1,4}+k_{2,4})}{(k_{3,2}+k_{4,2})} \left(\frac{(k_{1,4}+k_{2,4})k_{3,2}k_{2,1}}{(k_{3,2}+k_{4,2})k_{4,3}k_{1,4}}\right)^{-\frac{1}{3}} \\ x_4 &= z_4 \end{aligned}$$

is obtained where z_4 *is an arbitrary complex number. The parametrization is in the direction of the last row of* U *being* $(-1, 1, 2, 1)$ *which is orthogonal to im*$(YA) = S =$ *im*(Π). *Precisely one of the three roots is real and positive since all constants* k_{ij} *are positive. Choosing* $z_4 = x_4 \in \mathbf{R}_+$ *gives a family of positive solutions which intersects each space* $(x_0 + im(YA)) \cap (\mathbf{R}_+)^4$ *once.*

The following proposition uses the sparseness of the bipartite graph. For a vector $y \in \mathbf{R}^m$ we define the *support* $\mathrm{supp}(y) = \{i \in \{1, \ldots, m\} \mid y_i \neq 0\}$.

Proposition 4.3 *Let a chemical reaction system be given by its directed graph R, the weighted adjacency matrix K and the complexes $y_1, \dots, y_n \in (\mathbf{Z}_{\geq 0})^m$ as vertices forming the stoichiometric matrix $Y \in (\mathbf{Z}_{\geq 0})^{m,n}$. The kinetic matrix $A = K - diag(K^t e)$ together with the monomial mapping $\Psi : \mathbf{C}^m \to \mathbf{C}^n$, $x \mapsto (x^{y_1}, \dots, x^{y_n})$ defines the system $YA\Psi(x) = 0$. Let $\mathcal{L}_\lambda \subset \{1, \dots, n\}$, $\lambda = 1, \dots, l$ be the connected components of R and $\mathcal{T}_\nu^\lambda, \nu = 1, \dots, t_\lambda, t_1 + \dots + t_l = t$ its terminal strong linkage classes. Let $\mathcal{T} = \bigcup_{\lambda=1}^l \bigcup_{\nu=1}^{t_\lambda} \mathcal{T}_\nu^\lambda$ be the terminal part and $\mathcal{R} = \{1, \dots, n\} \setminus \mathcal{T}$ the rest. Assume*

$$rank(YA) = rank(A).$$

If $y_i \neq \mathbf{0}$ for all $i \in \mathcal{R}$ then the complex solutions $x \in \mathbf{C}^m$ of $YA\Psi(x) = 0$ are of the following form

a.) There exists an index set I with $x_i \neq 0$ for $i \in \{1, \dots, m\} \setminus I$ and $x_i = 0$ for all $i \in I$ and an index set $\mathcal{A} = \{(\lambda, \nu) \mid \lambda \in \{1, \dots, l\}, \nu \in \{1, \dots, t_\lambda\},\}$ such that

- *i.) $supp(y_j) \cap I \neq \emptyset$ for all $j \in \mathcal{R}$,*
- *ii.) $supp(y_j) \cap I = \emptyset$ for all $j \in \mathcal{T}_\nu^\lambda$ for all $(\lambda, \nu) \in \mathcal{A}$,*
- *iii.) $supp(y_j) \cap I \neq \emptyset$ for all $j \in \mathcal{T}_\nu^\lambda$ for all $(\lambda, \nu) \notin \mathcal{A}$.*

b.) The solutions with $m - |I|$ remaining coordinates x_i come in families, each depending on $m - |I| - q$ free parameters where $q = |\mathcal{B}| - |\mathcal{A}|$ is the rank of the matrix $(a_{\mu\sigma}), \mu, \sigma \in \mathcal{B}$ where $\mathcal{B} = \bigcup_{(\lambda,\nu) \in \mathcal{A}} \mathcal{T}_\nu^\lambda$.

c.) Define $J = span(\omega_i, i \notin I) \subset \mathbf{C}^m$, $\tilde{P}P : \mathbf{C}^m \to \mathbf{C}^m$, $(\tilde{P}Py)_i = 0, i \in I$, $(\tilde{P}Py)_i = y_i, i \notin I$, and $V = span(\{\tilde{P}P(y_i - y_j) \mid i, j \in \mathcal{T}_\nu^\lambda, (\lambda, \nu) \in \mathcal{A}\})$. Each family intersects within $J \cap (\mathbf{R}_{\geq 0})^m$ for each $x_0 \in J$ the space $(x_0 + V) \cap (\mathbf{R}_{\geq 0})^m$ except of some coordinate hyperplanes. The intersection is transversal.

In particular, if the graph is not weakly reversible then there are no positive solutions.

Proof: Because rank(YA) =rank(A) it is sufficient to solve $A\Psi(x) = 0$. By Theorem 3.4 rank$(A) = n - t$ which yields $m \geq n - t$. The linear mapping $A : \mathbf{C}^n \to \mathbf{C}^n$ splits into $A_{|R} : R \to \mathbf{C}^n$ and $A_{|T} : T \to \mathbf{C}^n$ (with $R = \text{span}(\{\omega_i, i \in \mathcal{R}\})$, $T = \text{span}(\{\omega_i, i \in \mathcal{T}\})$) since $\mathbf{C}^n = R \oplus T$. Demanding $A_{|R} u = 0$ is equivalent to demanding $u_j = 0$ for all $j \in \mathcal{R}$ since $A_{|R}$ has maximal rank due to the positivity of the constants k_{ij}. This shows that the solutions have necessarily the property described in i.). We start with a minimal set I of indices with this property. Of course there may be several choices. By the minimality we have $|I| \leq |\mathcal{R}|$. Define $\mathcal{A} = \{(\lambda, \nu) \mid \lambda \in \{1, \dots, l\}, \nu \in \{1, \dots, t_\lambda\}\}$. For the $m - |I|$ remaining variables $X_i = x_{j_i}, j_i \in \{1, \dots, m\} \setminus I$ the system $A\Psi(\tilde{P}X) = 0$ is a smaller system of equations where $X = (x_{i_1}, \dots, x_{i_{m-|I|}})$, $i_1, \dots, i_{m-|I|} \in \{1, \dots, m\} \setminus I$ and $\tilde{P}$ fills up with zeros. Here $X = Px$ and P denotes the projection from $\mathbf{C}^m$ to $\mathbf{C}^{m-|I|}$ while $\tilde{P}$ is the embedding of $\mathbf{C}^{m-|I|}$ into $\mathbf{C}^m$. Since the monomials x^{y_j} for $j \in \mathcal{R}$ and for $j \in \mathcal{T}$ with supp$(y_j) \cap I \neq \emptyset$ are zero the equations are restricted to $QA_{|B}\tilde{\Psi}(\tilde{P}X) = 0$

with $\mathcal{B} = \{i \in \mathcal{T} \,|\, \mathrm{supp}(y_i) \cap I = \emptyset\}$ and $B = \mathrm{span}(\{\omega_i, i \in \mathcal{B}\})$ and $Q : \mathbf{C}^m \to T$ a projection onto T and $\tilde{\Psi} : \mathbf{C}^m \to \mathbf{C}^{|\mathcal{B}|}$ the collection of monomials associated to $\mathcal{B}$. Recall from Lemma 3.3 that A is invariant on each terminal strong linkage class $\mathcal{T}_\nu^\lambda$ or its corresponding vector space T_ν^λ, respectively. Moreover, by Theorem 3.4 we deduce that $x^{y_j} = 0$ for all $j \in \mathcal{T}_\nu^\lambda$ or $\mathrm{supp}(y_j) \cap I = \emptyset$ for all $j \in \mathcal{T}_\nu^\lambda$. In order to satisfy the first condition one might need to enlarge I. Redefine $\mathcal{A}, \mathcal{B}, P, \tilde{P}, Q, \tilde{\Psi}$ and consider $QA_{|B}\tilde{\Psi}(\tilde{P}X) = 0$ again. After a finite number of repetitions this process terminates. This gives the index sets $\mathcal{A}$ and I such that $x_i = 0, \forall\, i \in I, x^{y_j} = 0, j \in \mathcal{T}_\nu^\lambda, (\lambda, \nu) \in \mathcal{A}$. It remains to solve

$$\begin{pmatrix} A_{ij} & & 0 \\ & \ddots & \\ & & A_{kl} \end{pmatrix} \tilde{\Psi}(PX) = 0,$$

where only block $A_{\lambda\nu}$ with $(\lambda, \nu) \in \mathcal{A}$ appear. By Theorem 3.4 linear transformation gives a system

$$X^{\pi_1} = c_1, \quad \ldots \quad , X^{\pi_q} = c_q, \tag{3}$$

with constants $c_i \in \mathbf{R}_+$ and $\pi_k = P(y_i - y_j)$ for some oriented edge $C_j \to C_i$ in a terminal strong linkage class $\mathcal{T}_\nu^\lambda$ with $(\lambda, \nu) \in \mathcal{A}$ and thus $\mathrm{supp}(y_j) \cap I = \emptyset$, $\mathrm{supp}(y_i) \cap I = \emptyset$. As in the proof of Theorem 4.1 we use the Smith normal form. A matrix $\Pi \in (\mathbf{Z})^{p,q}$ is formed by the π_k as columns where $p := m - |I|$ and q is the rank of Π. Observe that q is as well the rank of the remaining coefficient matrix $(a_{\mu\sigma})_{\mu\sigma\in\mathcal{B}}$. We know $p = m - |I| \geq n - t - |\mathcal{R}| - \sum_{(\lambda,\nu)\notin\mathcal{A}}(|\mathcal{T}_\nu^\lambda| - 1) = |\mathcal{B}| - |\mathcal{A}| = q$. Thus all invariant factors $s_j \in \mathbf{N}$ in the Smith normal form

$$U \Pi V = \begin{pmatrix} s_1 & & 0 \\ & \ddots & \\ 0 & & s_q \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad U \in GL(p, \mathbf{Z}), V \in GL(q, \mathbf{Z}) \quad s_j | s_{j+1}, j = 1, \ldots, q-1\,,$$

are non-zero. System (3) is then solved by a nonlinear change of coordinates

$$X_1 = z_1^{u_{11}} \cdots z_p^{u_{p,1}}, \quad \ldots \quad , X_p = z_1^{u_{1,p}} \cdots z_p^{u_{p,p}}. \tag{4}$$

Substitution into (3) and manipulation involving V results in a system

$$z_1^{s_1} = c_1', \quad \ldots \quad , z_q^{s_q} = c_q'\,. \tag{5}$$

The constants $c_i' \in \mathbf{R}_+$ are positive since $c_i' = \prod_{j=1}^q c_j^{v_{ji}}$. This determines $z_1, \ldots, z_q$ and $z_{q+1}, \ldots, z_p$ remain arbitrary complex numbers. The number of solution families is $\prod_{i=1}^q s_i = \det(\Pi)$.

Now we proof part c.). Since $s_1, \ldots, s_q$ are the invariant factors the variables $z_1, \ldots, z_q$ form a nonlinear parametrization of $\mathrm{im}(\Pi)$. Given a solution $z \in (\mathbf{R}_+)^p$ the perturbation

$$(z_1, \ldots, z_q, z_{q+1} + \delta z_{q+1}, \ldots, z_p + \delta z_p)$$

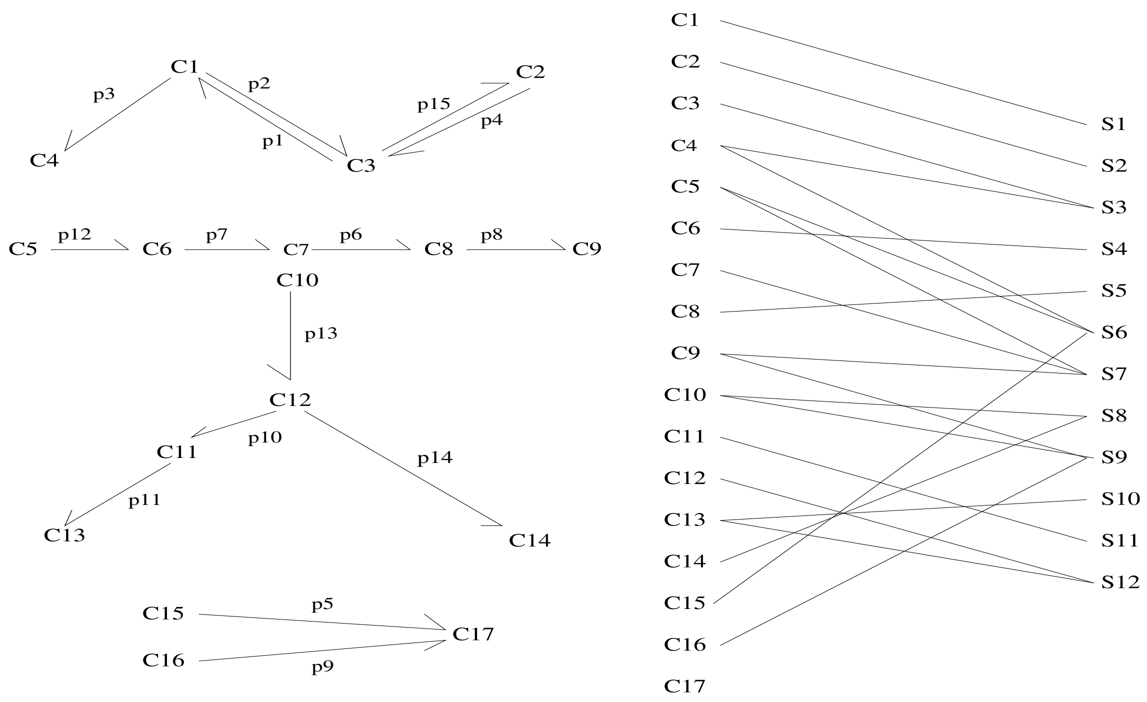

Figure 6: Enzyme synthesis in a bacteriell cell (Heinmets).

is in a direction transversal to $X_0 + \mathrm{im}(\Pi)$. The corresponding families within $(\mathbf{R}_{\geq 0})^m$ are transversal to $(\tilde{P}X_0 + \tilde{P}\,\mathrm{im}(\Pi)) \cap (\mathbf{R}_{\geq 0})^m$. The number of parameters equals $p - q = m - |I| - |\mathcal{B}| + |\mathcal{A}|$. All classes are intersected except of some coordinate hyperplanes. The exception is due to the fact that some exponents in (4) are positive and some are negative such that a limit $z_i \to 0$ for some $i \in \{q+1, \ldots, p\}$ results in some limit $X_j \to \infty$ and some $X_k \to 0$. □

Part of the statement of Proposition 4.3 can be formulated more general.

Lemma 4.4 *Consider the system $YA\Psi(x) = 0$ as in Proposition 4.3 and the notations therein. Assume that the directed graph is not weakly reversible and there exist an index $i \in \mathcal{R}$ such that Ya_i is linear independent of the other columns $Ya_j, j \in \{1, \ldots, m\} \setminus \{i\}$. If $y_i \neq \mathbf{0}$ then the system $YA\Psi(x) = 0$ has no solutions in $(\mathbf{C}^*)^m$. 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 an equation $x^{y_i} = 0$ has to be satisfied. If $y_i \neq \mathbf{0}$ this can be only satisfied if some component $x_j = 0$ where $j \in \mathrm{supp}(y_i)$. The case $y_i = \mathbf{0}$ yields the unsolvable equation $1 = 0$. □

Example 4.5 *A model introduced by Heinmets (see also [2] and [21]) 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 this inducer* S_3 *and a* functional gene S_7 *and a* ribosome S_8 *are present. Since in [2] and [21] only the differential equations are given we constructed a directed graph and a bipartite graph as in Figure 6 such that these equations result. The stoichiometric matrix is*

$$Y = \begin{bmatrix} 1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0 \\ 0&0&0&1&1&0&0&0&0&0&0&0&0&0&1&0&0 \\ 0&0&0&0&1&0&1&0&1&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&1&0&0&0&1&0&0&0 \\ 0&0&0&0&0&0&0&0&1&1&0&0&0&0&0&1&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&1&1&0&0&0&0 \end{bmatrix}$$

and the kinetic matrix is

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

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

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

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

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

The described differential equations are

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

Since rank$(A_3) =$ *rank*$(Y3A_3) = 3$ *and rank*$(YA) = 9$, *but rank*$(Y1A_1, Y_2A_2, Y_4A_4)) = 6$ *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*

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

Obviously, we need to consider two cases.
1. Case $(x_8 = x_{11} = x_{12} = 0)$*: Substitution gives the remaining equations*

$$
\begin{aligned}
(-p_2 - p_3)\, x_1 + p_1 x_3 &= 0 \\
-p_4 x_2 + p_{15} x_3 &= 0 \\
(p_2 + p_3)\, x_1 + p_4 x_2 + (-p_1 - p_{15})\, x_3 &= 0 \\
p_{12} x_6 x_7 - p_7 x_4 &= 0 \\
p_6 x_7 - p_8 x_5 &= 0 \\
p_3 x_1 - p_{12} x_6 x_7 - p_5 x_6 &= 0 \\
-p_{12} x_6 x_7 + p_7 x_4 - p_6 x_7 + p_8 x_5 &= 0 \\
p_8 x_5 - p_9 x_9 &= 0
\end{aligned}
$$

This are 7 linear equations in 9 monomials. A solution is obviously

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

2. Case $(x_9 = x_{11} = x_{12} = 0)$*: Substituting this restriction into the polynomial equations yields the equations* $p_8 x_5 = 0$. *Subsitution of* $x_5 = 0$ *gives the equation* $x_7 = 0$ *and then* $x_4 = 0$. *The remaining equations are*

$$
\begin{aligned}
(-p_2 - p_3)\, x_1 + p_1 x_3 &= 0 \\
-p_4 x_2 + p_{15} x_3 &= 0 \\
(p_2 + p_3)\, x_1 + p_4 x_2 + (-p_1 - p_{15})\, x_3 &= 0 \\
p_3 x_1 - p_5 x_6 &= 0.
\end{aligned}
$$

A solutions is obviously

$$x_1 = \frac{p_5 x_6}{p_3}, \quad x_2 = \frac{p_{15} p_5 x_6 \, (p_2 + p_3)}{p_4 p_1 p_3}, \quad x_3 = \frac{p_5 x_6 \, (p_2 + p_3)}{p_3 p_1}.$$

These solutions have been computed in [21] using Göbner bases in the ring $Q(p)[x]$. But this derivation shows that nothing complicated is necessary. Already pour linear algebra gives the result.

5 Exploiting the sublattice

The result of the last section heavily depends on the fact that the exponents of the monomials are $y_i - y_j$ with $i, j \in \mathcal{L}_\lambda$ in the same connected component. The following lemma is similiarly based on the structure of the sublattice induced by the two graphs. A hint to this lemma may be found in [9] p. 2262.

Lemma 5.1 *Consider the system $YA\Psi(x) = 0$ induced by the two graphs. Assume that the directed graph is weakly reversible and*

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

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

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

are collection of columns and rows corresponding to connected components, respectively. Then each $(x_0 + im(YA)) \cap (\mathbf{R}_+)^m$ contains the same number of real positive solutions of $YA\Psi(x) = 0$.

Proof: Because of (6) the system $YA\Psi(x) = 0$ is equivalent to

$$\sum_{j\in\mathcal{L}_\lambda} a_{ij}\, x^{y_j} = 0, \quad i \in I_\lambda \subset \mathcal{L}_\lambda, \quad \lambda = 1, \ldots, l\,,$$

for some index set $I_\lambda \subset \mathcal{L}_\lambda$ with cardinality $\text{rank}(Y_\lambda A_\lambda)$. In order to see this build for each $\lambda = 1, \ldots, l$ the orthogonal complement of $\text{span}(Y_1 A_1 \cdots \widehat{Y_\lambda A_\lambda} \cdots Y_l A_l))$ in $\text{im}(YA)$ and multiply a vector space basis of the complement with YA. Here $\widehat{Y_\lambda A_\lambda}$ means to leave out this matrix.

For each equation with index i we choose a monomial $y^{\nu(i)}$ and get

$$\sum_{j\in\mathcal{L}_\lambda\setminus\{\nu(i)\}} a_{ij}\, x^{y_j - y_{\nu(i)}} = -a_{i\nu(i)}, \quad i \in I_\lambda, \quad \lambda = 1, \ldots, l\,.$$

Since $y_j - y_{\nu(i)}$ are generators of the stoichiometric space S and $S = \text{im}(YA)$ because of the weak reversibility of the directed graph the lattice generated by the monomials in the equations has dimension $\text{rank}(YA) = \dim(S) = s$. By Smith normal form (see [1] p. 325) we may find generators $x^{\alpha_1}, \ldots, x^{\alpha_s}$ and $x^{\gamma_1}, \ldots, x^{\gamma_{m-s}}$ such that $\alpha_1, \ldots, \alpha_s, \gamma_1, \ldots, \gamma_{m-s}$ are linear independent over $\mathbf{C}$ and such that $\alpha_1, \ldots, \alpha_s$ generate a lattice of dimension s and $\gamma_1, \ldots, \gamma_{m-s}$ give transversal directions. A coordinate transformation $z_1 = x^{\alpha_1}, \ldots, z_s = x^{\alpha_s}$, $v_1 = x^{\gamma_1}, \ldots, v_{m-s} = x^{\gamma_{m-s}}$ results in a polynomial system

$$\sum_{j \in \mathcal{L}_\lambda \setminus \{\nu(i)\}} a_{ij}\, z^{\delta_j} = -a_{i\nu(i)}, \quad i \in I_\lambda, \quad \lambda = 1, \ldots, l,$$

with some $\delta_j \in (\mathbf{Z}_{\geq 0})^s$. Also the number of equations equals the number of variables s. The polynomial system is independent of the variables $v_1, \ldots, v_{m-s}$ which gives a nonlinear parametrization of the space transversal to $\mathrm{im}(YA)$.

This transformation is performed in the following way: Collect the $y_j - y_{\nu(i)}$ as columns of a matrix B and compute the Smith normal form UBV.

Then $U^{-1} = (\alpha_1, \ldots, \alpha_s, \gamma_1, \ldots, \gamma_{m-s})$ and

$$UB = \begin{pmatrix} * & \cdots & * & \cdots & * \\ & \ddots & * & \vdots & * \\ 0 & & * & \cdots & * \\ & 0 & \cdots & 0 & \end{pmatrix}$$

contains the exponents δ_j as columns plus additional zeros.

A solution x is positive if and only if z, v are positive. An argumentation analogous to the proof of the deficiency zero theorem yields that each affine space $x_0 + \mathrm{im}(YA)$ contains exactly the same number of real positive solutions. $\square$

In the lemma the sublattice has a very nice property. If the directed graph is not weakly reversible or the rank condition (6) is violated then the sublattice has dimension larger than $\dim(\mathrm{im}(YA))$. Most likely the dimension is m. But in some special cases it is still possible to make statements about directions transversal to the variety.

Lemma 5.2 *Let the connected component $\mathcal{L}_\lambda$ equal its terminal strong linkage class for some $\lambda \in \{1, \ldots, l\}$ and assume rank(A_λ) = rank$(Y_\lambda A_\lambda)$, rank(YA) = rank$(Y_\lambda A_\lambda)$ + rank$(Y_1 A_1 \cdots \widehat{Y_\lambda A_\lambda} \cdots Y_l A_l)$). If the variety of $YA\Psi(x) = 0$ intersects $(x_0 + im(Y_\lambda A_\lambda)) \cap (\mathbf{R}_+)^m$ for some $x_0 \in \mathbf{R}^m$ then it intersects transversally. Each $(x_0 + im(Y_\lambda A_\lambda)) \cap (\mathbf{R}_+)^m$ contains at most one positive solution.*

Proof: $Y_\lambda A_\lambda \Psi(x) = 0$ is equivalent to a binomial system $x^{y_i - y_{\nu(j)}} = c_j, j = 1, \ldots, |\mathcal{L}_\lambda| - 1$ with positive constants c_j and $i, \nu(j) \in \mathcal{L}_\lambda$. The exponents $y_j - y_{\nu(j)}$ are elements of $\mathrm{im}(Y_\lambda A_\lambda)$. Then the argumentation is analogous to the deficiency zero theorem. $\square$

Lemma 5.3 *Let the connected component $\mathcal{L}_\lambda$ equal its terminal strong linkage class for one $\lambda \in \{1, \ldots, l\}$ and assume*

$$\mathit{rank}(YA) = \mathit{rank}(Y_\lambda A_\lambda) + \mathit{rank}((Y_1 A_1 \cdots \widehat{Y_\lambda A_\lambda} \cdots Y_l A_l)).$$

Then the system $YA\Psi(x)=0$ decouples into two polynomial systems. If the variety of solutions of $YA\Psi(x)=0$ intersects $(x_0+im(Y_\lambda A_\lambda))\cap(\mathbf{R}_+)^m$ then it intersects transversally. Each solution in

$$(x_0+M_1+M_2+im(YA))\cap(\mathbf{R}_+)^m \quad \textit{where}$$

$$\begin{aligned} M_1 = span\{y_i-y_j \mid \quad & i\in\mathcal{L}_\mu\, j\in\mathcal{L}_\nu, \mu\neq\lambda, \nu\neq\lambda, \mu\neq\nu, \\ & rank(Y_\mu A_\mu, Y_\nu A_\nu)) < rank(Y_\mu A_\mu) + rank(Y_\nu A_\nu)\ \}, \\ M_2 = span\{y_i-y_j \mid \quad & i\in\mathcal{L}_\mu\, j\in\mathcal{L}_\nu, \mu\neq\lambda, \nu\neq\lambda, \mu\neq\nu, \\ & rank(Y_\mu A_\mu, Y_\nu A_\nu)) = rank(Y_\mu A_\mu) + rank(Y_\nu A_\nu) \\ & rank(YA) < rank((Y_1A_1,\ldots,\widehat{Y_\mu A_\mu},\ldots,\widehat{Y_\nu A_\nu},\ldots,Y_lA_l))+ \\ & \qquad rank(Y_\mu A_\mu)+rank(Y_\nu A_\nu)\ \} \end{aligned}$$

belongs to a family of positive solutions of $YA\Psi(x)=0$ which intersects transversally $x_0+M_1+M_2+im(YA)$. Each family intersects each $(x_0+M_1+M_2+im(YA))\cap(\mathbf{R}_+)^m$.

Proof: Because of the rank condition $YA\Psi(x)=0$ is equivalent to $Y_\lambda A_\lambda\tilde{\Psi}(x)=0$ and $Y_1A_1\cdots\mathbf{0}\cdots Y_lA_l)\Psi(x)=0$. The first is equivalent to

$$\sum_{j\in\mathcal{L}_\lambda\setminus\{\nu(i)\}} a_{ij}x^{y_j-y_{\nu(i)}} = a_{i\nu(i)}, \quad i\in I_\lambda\subset\mathcal{L}_\lambda,$$

for some index set $I_\lambda\subset\mathcal{L}_\lambda$ with cardinality $|I_\lambda| = \mathrm{rank}(Y_\lambda A_\lambda)$ and some $\nu(i)\in I_\lambda$. Since the connected component is a terminal strong linkage class the occuring exponents generate a lattice of dimension $\mathrm{rank}(Y_\lambda A_\lambda)=|I_\lambda|=r$. Let's assume that the sublattice is generated by $\alpha_1,\ldots,\alpha_r\in\mathbf{Z}^m$. The second group of equations give raise to a lattice genrated by vectors M_1, M_2 and $\mathrm{im}(YA)$. So complete the α_i by $\beta_1,\ldots,\beta_d$ to a basis of this second lattice of dimension $d=\dim(M_1+M_2+\mathrm{im}(YA)$. Then $\gamma_1\ldots,\gamma_{m-r-d}$ complete to a basis of $\mathbf{Z}^m$. A change of coordinates $z_1=x^{\alpha_1},\ldots,z_r=x^{\alpha_r}$, $u_1=x^{\beta_1},\ldots,u_d=x^{\beta_d}$, $v_1=x^{\gamma_1},\ldots,v_{m-r}=x^{\gamma_{m-r-d}}$ gives r polynomials in r variables $z_1,\ldots,z_r$ only. Additionally, there are $\mathrm{rank}(YA)-r$ polynomials in $r+d$ variables $z_1,\ldots,u_d$. For each solution z of the first system there may be several families of solutions of the second system. The remaing statements of the theorem follow analogous to the argumentation in the proof of the deficiency zero theorem. □

6 More binomial cases

Feinberg formulates in [8, 9, 10] a theorem which he calls the *deficiency one theorem.* The assumptions in [10] are more restrictive then in [8]. We give here our version.

Theorem 6.1 *Consider the system $YA\Psi(x)=0$ of polynomial equations defined by a directed graph with weighted adjacency matrix K and a bipartite graph with relevant part Y of the weighted adjacency matrix and $A=K-diag(K^te)$. Assume that each connected* *components $\mathcal{L}_\lambda$ of the directed graph contains only one terminal strong linkage class $\mathcal{T}_1^\lambda$. Assume*

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

where $A = (a_{ij}), A_\lambda = (a_{ij})_{i=1,j\in\mathcal{L}_\lambda}$, $Y_\lambda = (y_{ij})_{i=1,\dots,n,j\in\mathcal{L}_\lambda}$. Assume rank(span($Ya_i, i \in \mathcal{T}_1^\lambda$)) $= |\mathcal{T}_1^\lambda| - 1$ for each $\lambda \in \{1,\dots,l\}$ and for the rests $\mathcal{R}_\lambda = \mathcal{L}_\lambda \setminus \mathcal{T}_1^\lambda$ either $Ya_i \in$ span($Ya_j, j \in \mathcal{T}_1^\lambda$) for all $i \in \mathcal{R}_\lambda$ or rank($Ya_i, i \in \mathcal{R}_\lambda$) $= |\mathcal{R}_\lambda| - 1$ and none of the Ya_i is linear independent of the other $Ya_j, j \in \mathcal{R}_\lambda \setminus \{i\}$. Then each class $(x_0 + im(YA)) \cap (\mathbf{R}_+)^m$ contains precisely one positive real solution.

Proof: The conditions on the ranks and components assure that $YA\Psi(x) = 0$ is equivalent to a binomial system. Since each component contains only one terminal strong linkage class this yields $\mathrm{im}(YA) = S$. Using the Smith normal form the argumentation is analogous to the deficiency zero theorem. □

Theorem 6.2 *(Deficiency One Theorem, Feinberg [9] p. 2259, proof in [12]) Let the graph be weakly reversible and rank($Y_\lambda A_\lambda$) $\geq |\mathcal{L}_\lambda| - 2$ for each connected component for $\lambda = 1,\dots,l$. Moreover, assume*

$$\textit{rank}(YA) = \sum_{\lambda=1}^{l} \textit{rank}(Y_\lambda A_\lambda). \tag{7}$$

Then each space $(x_0 + S) \cap (\mathbf{R}_+)^m$ contains precisely one real positive solution.

Proof: Because of the assumption (7) on the rank the polynomial system decouples as stated in Lemma 5.3. Thus we may assume that the graph has one connected component only with $\mathrm{rank}(YA) = \mathrm{rank}(A) - 1 = n - 2$. By Lemma 5.1 it is clear that each space $x_0 + \mathrm{im}(YA)$ contains the same number of positive solutions. It remains to show the existence of precisely one solution.

First we consider the Hermite normal form of Y. Since $\mathrm{rank}(YA) = \mathrm{rank}(A) - 1$ we may assume the shape

$$H := UY = \begin{pmatrix} h_{1,1} & & & \cdots & h_{1,i-1} & h_{1,i} & h_{1,i+1} & \cdots & h_{1,n} \\ 0 & h_{2,2} & & \cdots & h_{2,i-1} & h_{2,i} & h_{2,i+1} & \cdots & h_{2,n} \\ 0 & 0 & h_{3,3} & & \vdots & \vdots & \vdots & & \vdots \\ & & & \ddots & \vdots & \vdots & \vdots & & \vdots \\ & & & & h_{i-1,i-1} & h_{i-1,i} & & & \\ \vdots & & & & 0 & 0 & h_{i,i+1} & & \vdots \\ & & & & & & & \ddots & \\ 0 & & & & \cdots & & & 0 & h_{n-1,n} \\ 0 & & & & \cdots & & & & 0 \end{pmatrix},$$

where $U \in GL(n,\mathbf{Z})$ and diagonal elements $h_{11}, h_{22}, \dots, h_{i-1,i-1}, h_{i,i+1}, \dots, h_{n-1,n} \in \mathbf{N}$ are integer numbers and $h_{kl} \in \mathbf{Z}_{\geq 0}, h_{kl} < h_{ll}$ for $l = 2,\dots,i-1, 1 \leq k < l$ or $h_{kl+1} \in$

$\mathbf{Z}_{\geq 0}, h_{kl+1} < h_{l,l+1}$ for $l = i, \ldots, n-1, 1 \leq k < l$. The i-th column simply consists of integer numbers. We may perform a nonlinear change of coordinates $x = z^U$ such that the exponents of the monomials are $Uy_1, Uy_2, \ldots, Uy_n$. Then the system reads

$$HA\,m(z) = HA \begin{pmatrix} & & & & & z_1^{h_{1,1}} \\ & & & & z_1^{h_{1,2}} & z_2^{h_{2,2}} \\ & & & z_1^{h_{1,3}} & z_2^{h_{2,3}}. & z_3^{h_{3,3}} \\ & & & & & \vdots \\ & z_1^{h_{1,i-1}} & z_2^{h_{2,i-1}} & z_3^{h_{3,i-1}} & \cdots & z_{i-1}^{h_{i-1,i-1}} \\ z_1^{h_{1,i}} & z_2^{h_{2,i}} & z_3^{h_{3,i}} & z_4^{h_{4,i}} & \cdots z_{i-1}^{h_{i-1,i}} & \\ & z_1^{h_{1,i+1}} & z_2^{h_{2,i+1}} & z_3^{h_{3,i+1}} & \cdots & z_i^{h_{i,i+1}} \\ & & & & & \vdots \\ z_1^{h_{1,n-1}} & z_2^{h_{2,n}} & z_3^{h_{3,n}} & \cdots & z_{n-2}^{h_{n-2,n}} & z_{n-1}^{h_{n-1,n}} \end{pmatrix} = 0.$$

We have $n-1$ variables $z_1, \ldots, z_{n-1}$, but n monomials. The monomials satisfy the relation

$$(m_1(z))^{g_1}(m_2(x))^{g_2} \cdots (m_i(x))^{g_i} = 1,$$

with an element $g = (g_1, \ldots, g_i, 0) \in \operatorname{kernel}(Y) \cap \mathbf{Z}^n$. So each $u \in \operatorname{kernel}(YA)$ with $u_1^{g_1} u_2^{g_2} \cdots u_i^{g_i} = 1$ gives a solution since $m(z) = u$ is easily solved by backward substitution. If u is positiv this gives a positiv solution z which is equivalent to a positiv x in the original coordinates.

Thus we study positive kernel vectors of HA. The first part is $\operatorname{kernel}(A)$ which is generated by one $a \in (\mathbf{R}_+)^n$ because of the special structure of A. Since $\dim(\operatorname{kernel}(YA)) = 2$ we choose a second linear independent vector b in $\operatorname{kernel}(YA)$. Since a is strictly positiv we choose one $b \in (\mathbf{R}_{\geq 0})^n$ such that at least one component b_j is zero. Secondly, we may find a vector $c \in (\mathbf{R}_{\geq 0})^n$ in the kernel of $\operatorname{kernel}(YA)$ with at least one component $c_k = 0$. Now we study all $\lambda b + \mu c$ with $\lambda > 0, \mu > 0$ which satisfy

$$(\lambda b_1 + \mu c_1)^{g_1}(\lambda b_2 + \mu c_2)^{g_2} \cdots (\lambda b_i + \mu c_i)^{g_i} - 1 = 0.$$

The goal is to show that for each given positiv λ there exists precisely one positiv μ fullfilling the equation. 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 take into account that some components of b, c are zero. Let $\omega_{supp(b)} = \sum_{i \in supp(b)} \omega_i$ and $\omega_{supp(c)} = \sum_{i \in supp(c)} \omega_i$ be vectors with entry one for each index of the support. Then

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

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

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

which yields

$$\omega_{supp(b)} Ab = (- \ \cdots \ - \ *_j \ - \ \cdots \ -) \ b < 0,$$

because A is negativ 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 [12] Lemma 8.1.4).

It is convenient to collect the positiv and negativ parts of g and to investigate the equivalent polynomial equation

$$f(\lambda, \mu) = (\lambda b + \mu c)^{g_+} - (\lambda b + \mu c)^{g_-} = 0, \tag{8}$$

where $\mathrm{supp}(g_+) \dot\cup \mathrm{supp}(g_-) \subseteq \{1, \ldots, i\}$. By the previous considerations we may assume

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

For given $\lambda_0 > 0, \mu_0 > 0$ with $f(\lambda_0, \mu_0) > 0$ we may find a large μ_1 with $f(\lambda_0, \mu_1) < 0$ because of the degree in the second monomial is larger. Obviously, there exists $\mu_2 \in (\mu_0, \mu_1)$ with $f(\lambda_0, \mu_2) = 0$. If we start with $f(\lambda_0, \mu_0) < 0$ we find a large λ_1 with $f(\lambda_1, \mu_0) > 0$ since the degree of the first monomial in λ is larger. Then $\lambda_2 \in (\lambda_0, \lambda_1)$ with $f(\lambda_1, \mu_0) = 0$ exists. The real variety also passes through $(0, 0)$. Since the derivatives $\frac{\partial f}{\partial \lambda} f(\lambda, \mu), \frac{\partial f}{\partial \mu} f(\lambda, \mu)$are nonzero there exists a solution for each λ. Because f consists of two monoton functions there is precisely one component of solutions.

If $e^t = (1, \ldots, 1)$ is a linear combination of the rows of Y, then $e^t g = 0$. Then f is homogeneous and the solutions $\lambda b + \mu c$ form half of a line. □

This proof reflects nicely the standard techniques for investigation of sparse polynomial systems. Usually, a system of linear equations is investigated on a toric variety. Our case is especially simple since the toric variety is defined by one polynomial $u^{g_+} - u^{g_-}$.

Example 6.3 *In [8] Feinberg illustrates the theorem with Example 3D1 on page 3-29. We recall the directed graph and the complexes in Figure 7. The equations are*

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

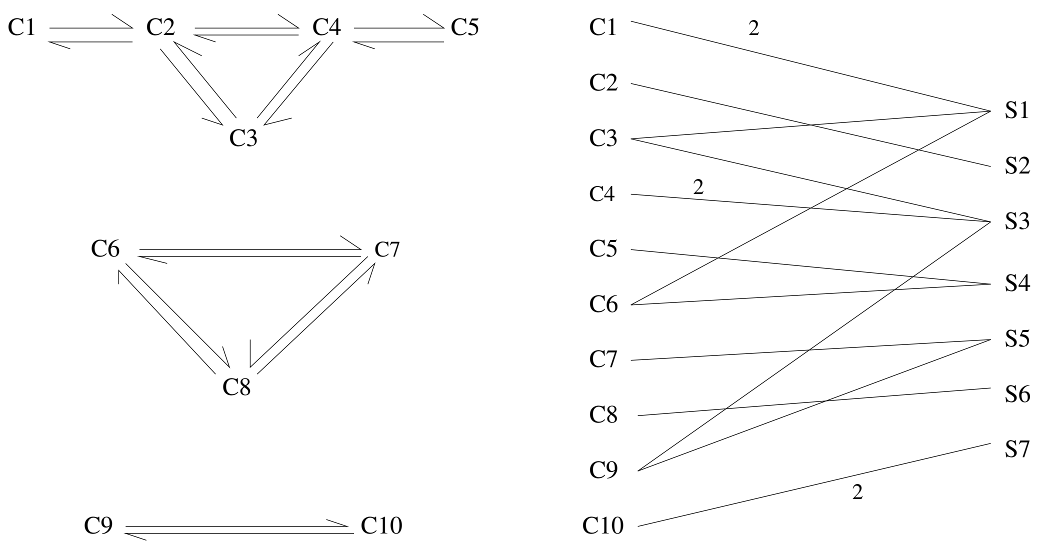

Figure 7: Example by Feinberg illustrating the assumptions in the Deciciency One Theorem.

The weakly reversible graph has three connected components such that the blocks of YA do not interact and rank$(Y_1A_1) = 3 < 4 =$ *rank*(A_1), *rank*$(Y_2A_2) = 2$, *and rank*$(Y_3A_3) = 1$.

After computing the Hermite normal form of Y and some linear algebra on HA we receive the polynomial system

$$\begin{pmatrix} H_1A_1 & & 0 \\ & H_2A_2 & \\ 0 & & H_3A_3 \end{pmatrix} \begin{pmatrix} \tilde{\Psi}_1(x) \\ \tilde{\Psi}_2(x) \\ \tilde{\Psi}_3(x) \end{pmatrix} = 0, \qquad \textit{with}$$

$$H_1A_1 = \begin{bmatrix} 2 & 0 & 0 & -2 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -k_{2,1} & k_{1,2} & 0 & 0 & 0 \\ k_{2,1} & -k_{1,2} - k_{4,2} & 0 & k_{2,4} & 0 \\ 0 & 0 & -k_{4,3} & k_{3,4} & 0 \\ 0 & k_{4,2} & k_{4,3} & -k_{2,4} - k_{3,4} - k_{5,4} & k_{4,5} \\ 0 & 0 & 0 & k_{5,4} & -k_{4,5} \end{bmatrix},$$

$$\tilde{\Psi}_1 = \left[{x_1}^2,\ x_2,\ x_1x_3,\ {x_3}^2,\ x_4 \right],$$

$$H_2A_2 = \begin{bmatrix} k_{7,6} & -k_{6,7} - k_{8,7} & k_{7,8} \\ k_{8,6} & k_{8,7} & -k_{6,8} - k_{7,8} \end{bmatrix}, \quad \tilde{\Psi}_2 = \begin{bmatrix} x_1x_4 \\ x_5 \\ x_6 \end{bmatrix},$$

$$H_3A_3 = \begin{bmatrix} 2\,k_{10,9} & -2\,k_{9,10} \end{bmatrix}, \quad \tilde{\Psi}_3 = \begin{bmatrix} x_3x_5 \\ {x_7}^2 \end{bmatrix}.$$

The Hermite normal form suggests the change of coordinates yielding the new monomials

$$m(z) = ({z_1}^2,\ z_2,\ z_3,\ \frac{{z_3}^2}{{z_1}^2},\ z_4,\ z_1z_4,\ z_5,\ z_6,\ \frac{z_3z_5}{z_1},\ {z_7}^2).$$

The last equation $H_3A_3m_3(z) = 0$ *gives*

$$z_7 = \pm\frac{\sqrt{k_{9,10}z_1z_3z_5k_{10,9}}}{k_{9,10}z_1}.$$

The second block is easily solved as well

$$z_5 = \frac{z_1z_4\left(k_{6,8}k_{7,6} + k_{7,8}k_{7,6} + k_{8,6}k_{7,8}\right)}{k_{6,8}k_{6,7} + k_{6,8}k_{8,7} + k_{7,8}k_{6,7}}, \quad z_6 = \frac{z_1z_4\left(k_{6,7}k_{8,6} + k_{8,7}k_{7,6} + k_{8,7}k_{8,6}\right)}{k_{6,8}k_{6,7} + k_{6,8}k_{8,7} + k_{7,8}k_{6,7}}.$$

The last equation of $H_1A_1m_1(z) = 0$ *gives*

$$z_4 = \frac{k_{5,4}{z_3}^2}{{z_1}^2k_{4,5}}.$$

Now we proceed analogous to the proof of the deficiency one theorem. The kernels of H_1 *and* A_1 *are generated by*

$$g = [1, 0, -2, 1, 0], \quad a = [1, \frac{k_{2,1}}{k_{1,2}}, \frac{k_{3,4}k_{2,1}k_{4,2}}{k_{4,3}k_{2,4}k_{1,2}}, \frac{k_{2,1}k_{4,2}}{k_{2,4}k_{1,2}}, \frac{k_{5,4}k_{2,1}k_{4,2}}{k_{4,5}k_{2,4}k_{1,2}}],$$

respectively. Of course the monomials satisfy the relation

$$m^g = (z_1^2)^1(z_2)^0(z_3)^{-2}(z_1^{-2}z_3^2)^1(z_4)^0 - 1 = 0.$$

A second kernel vector of H_1A_1 *is given by*

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

which has positive components, too. The system $\lambda a + \mu b = \tilde{m}_1(z)$ *has a positive solution* $z(\lambda, \mu)$ *for each positive* λ *if the equation*

$$\begin{aligned} f(\lambda, \mu) &= (a_1\lambda + \mu b_1)\cdot(a_4\lambda + \mu b_4) - (a_3\lambda + \mu b_3)^2 \\ &= \lambda\cdot(a_4\lambda + \mu b_4) - (a_3\lambda + \mu b_3)^2 = 0, \end{aligned}$$

has a solution $\mu \in \mathbf{R}$ *such that all components of* $\lambda a + \mu b$ *are positive. For positive* μ *all components of* $\lambda a + \mu b$ *are positive. For* $\mu = -a_3\lambda/b_3$ *we have* $f(\lambda, \mu) > 0$. *Since* $\lim_{\mu\to\pm\infty} = -\infty$ *there are two real solutions* μ. *But they are distinguished by the sign of* $a_3\lambda + \mu b_3$. *The solution with negative sign is not valid. For the other solution also* $a_4\lambda + \mu b_4 > 0$ *since* $f(\lambda, \mu) = 0$ *implies* $a_4\lambda + \mu b_4 = (a_3\lambda + \mu b_3)^2/\lambda$. *Symbolic manipolation with Maple has shown that* $a_2\lambda + \mu b_2 > 0$ *and* $a_5\lambda + \mu b_5 > 0$ *as well.*
Finally, we receive

$$z_1 = \sqrt{\lambda}, \quad z_2 = \lambda a_2 + \mu, \quad z_3 = \lambda a_3 + \mu b_3.$$

7 The general case

In this section we will attack the system $YA\Psi(x) = 0$ in general form in contrast to the previous sections where we made restrictive assumptions. In order to do so we will make use of the theory based on Newton polytopes. Consequently, we suggest to transform by linear algebra to an equivalent system such that the Newton polytopes of the equations are as simple as possible.

We restrict to directed graphs which are weakly reversible and as in the previous sections we use the decompositions $Y_\lambda = (y_{ij})_{i=1,\dots,m, j\in\mathcal{L}_\lambda}$ and $A_\lambda = (a_{ij})_{i,j\in\mathcal{L}_\lambda}$. If the conditions of Lemma 5.3 are fulfilled the system decouples. So we may assume we already have 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 $\lambda = 1, \dots, l$. For each connected component $\mathcal{L}_\lambda, \lambda = 1, \dots, l$ we may choose k_λ equations

$$\sum_{j\in\mathcal{L}_\lambda} c_{ij}\, x^{y_j} = 0, \quad i = 1, \dots, k_\lambda, \quad \lambda = 1, \dots, l\,, \tag{9}$$

where $k_\lambda < \operatorname{rank}(Y_\lambda A_\lambda)$ is the maximal number of columns of $Y_\lambda A_\lambda$ which are linear independent of $\operatorname{im}(Y_1 A_1, \dots, \widehat{Y_\lambda A_\lambda}, \dots, Y_l A_l)$. The coefficients c_{ij} are given by some linear independent rows of $Y_\lambda A_\lambda$.

By linear algebra we obtain from $YA\Psi(x) = 0$ the mixed equations containing all monomials

$$\sum_{j=1}^{n} c_{ij}\, x^{y_j} = 0, \quad i = 1, \dots, k_{l+1}, \tag{10}$$

where $k_{l+1} = \operatorname{rank}(YA) - \sum_{\lambda=1}^{l} k_\lambda$. The coefficients $(c_{ij})_{j\in\mathcal{L}_\lambda}$ are linear combinations of rows of $Y_\lambda A_\lambda$ which are linear independent of the rows appearing as coefficients in (9).

Additionally, the restrictions to $(x_0 + \operatorname{im}(YA)) \cap (\mathbf{R}_+)^m$

$$v_i^t\, x - a_i = 0, \quad i = 1, \dots, k_{l+2} \tag{11}$$

where $k_{l+2} = m - \operatorname{rank}(YA)$ and the vectors $v_i \in \mathbf{R}^m$ form an orthonormal basis of the orthogonal complement of $\operatorname{im}(YA)$ in $\mathbf{R}^m$. The $v_i^t x_0 = a_i \in \mathbf{R}$ are arbitrary but fixed numbers, such that $(x_0 + \operatorname{im}(YA)) \cap (\mathbf{R}_+)^m \neq \emptyset$. We may even assume that the first $v_1, \dots, v_l$ form an orthogonal basis of $S^\perp$ and $v_{l+1}, \dots, v_{k_{l+2}} \in S \cap (\operatorname{im}(YA))^\perp$.

Studying the solutions of $YA\Psi(x) = 0$ in $x_0 + \operatorname{im}(YA)$ is equivalent to studying the system (9,10,11).

Remark 7.1 *i.) The number of equations in the secondary group (10) is usually small, just* $1, 2$ *or* 3. *The support is the collection of supports in (9). Sometimes one may even further distinguish the supports of the* k_{l+1} *equations in (10). ii.) The Newton polytopes are of particular structure. Partially, they are simplices. But the Minkowski sum can not be expected to have full dimension* m. *If the graph is weakly reversible the* *dimension of the Newton polytope associated to $\mathcal{L}_\lambda$ is* $\dim(im(Y_\lambda A_\lambda))$. *There is a chance that* $|\mathcal{L}_\lambda| - rank(Y_\lambda A_\lambda) - 1$ *points are inner points. But most likely all points y_i with $i \in \mathcal{L}_\lambda$ are vertices since the points y_i lie on coordinate hyperplanes. iii.) The supports of (11) are the vertices of simplices of dimension m or less.*

The results on the number of complex or real solutions of a sparse polynomial system are based on a *homotopy* $\mathcal{H}(t,x)$.

$$\begin{aligned}
\mathcal{H}(t,x)_{\lambda,i} &= \sum_{j\in\mathcal{L}_\lambda} c_{ij}\, t^{\omega_j^\lambda} x^{y_j} = 0, \quad i = 1,\dots,k_\lambda, \quad \lambda = 1,\dots,l\,, && (12)\\
\mathcal{H}(t,x)_{l+1,i} &= \sum_{j=1}^{n} c_{ij}\, t^{\omega_j^{l+1}} x^{y_j} = 0, \quad i = 1,\dots,k_{l+1}, && (13)\\
\mathcal{H}(t,x)_{l+2,i} &= \sum_{j=1}^{m} (v_i)_j\, t^{\omega_j^{l+2}} x_j - a_i t^{\omega_0^{l+2}} = 0. \quad i = 1,\dots,k_{l+2} && (14)
\end{aligned}$$

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

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

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

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

Definition 7.2 ([18], [30], [31]) *A* subdivision *of $\mathcal{A}$ is a collection $\mathcal{S} = \{C_1,\dots,C_r\}$ of r cells $C_j = (C_j^{(1)},\dots,C_j^{(l+2)})$ such that*

(a) $\dim(conv(C_j)) = m$ *for* $j = 1,\dots,r$,

(b) $C_j \cap C_k$ *is a common face of* C_j and *of* C_k *for all pairs* $C_j, C_k \in \mathcal{S}$,

(c) $\cup_{j=1}^r conv(C_j) = conv(\mathcal{A})$.

The subdivision is called mixed *if the additional property*

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

The subdivision is called fine mixed *if*

(e) $\sum_{\lambda=1}^{l+2} (\#(C_j^{(\lambda)}) - 1) = m$ *for all cells* $C_j \in \mathcal{S}$.

A mixed subdivision is called simple mixed, *if all mixed cells C_j, i.e.* $\dim(conv(C_j^{(\lambda)})) = k_\lambda$

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

holds.

The definition of mixed subdivision is important since $\sum_j vol(C_j)$ is the BKK bound

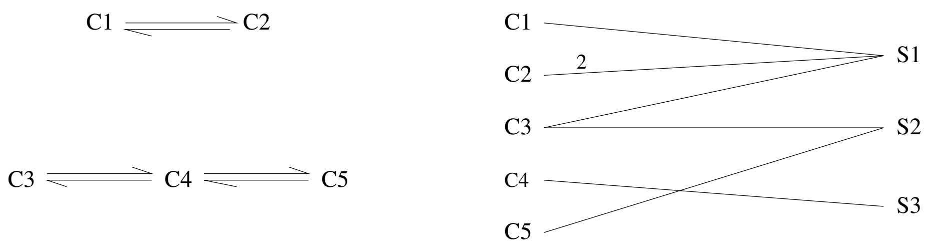

Figure 8: Example of a chemical reaction network by Feinberg due to Edelstein.

for the number of complex solutions in $(\mathbf{C}^*)^m$ (Theorem by Bernstein, see [4]). The proof in [18] gives some insight into the number of real solutions. But first we need another definition.

Definition 7.3 *A cell C is called* alternating *if the associated small initial system*

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

has exactly one positive solution.

This definition was introduced in [20] and [29] in the case that each equation has different support since then the small initial systems consists of binomials which obviously have one real solution if the signs of the coefficients are alternating in each equation.

Theorem 7.4 *[29] 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 have not infinitely many solutions for some $t \in [0,1]$ then the number of solutions of $YA\Psi(x) = 0$ in $(\sum_i a_i v_i + im(YA)) \cap (\mathbf{R}_+)^m$ equals the number of alternating cells in a mixed subdivision.*

The theoretical background may be found in [27], [29].

Remark 7.5 *i.) The polynomial $P(t)$ is the sparse resultant $Res_{\mathcal{B}}(t; k, a)$ 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 along the path. iii.) The condition whether a cell is alternating is easily chequed with Smith normal form or Hermite normal form for the mixed cells in a simple mixed subdivision. iv.) One expects that for generic lifting values ω_j^λ the induced subdivision is simple mixed. Since the Newton polytopes are not in general position in our particular application this cannot be expected for the chemical reaction systems.*

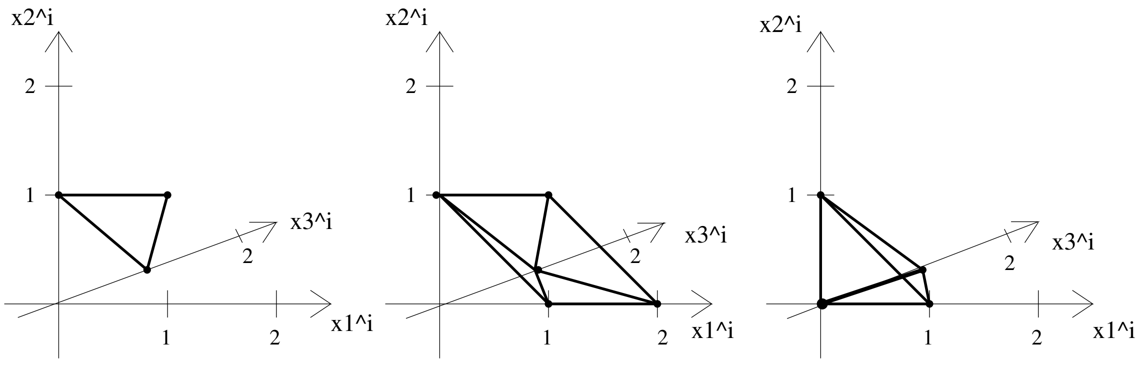

Figure 9: Newton Polytopes of system by Edelstein.

Example 7.6 *We illustrate Theorem 7.4 with the example by Edelstein presented in Feinberg [8] p.2-26 with* 3 *variables,* 5 *complexes and two connected components, see Figure 8.*

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

is the stoichiometric matrix and the kinetic matrix is

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

The 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 space $(av_1 + im(YA)) \cap \mathbf{R}^3$ is nonempty.

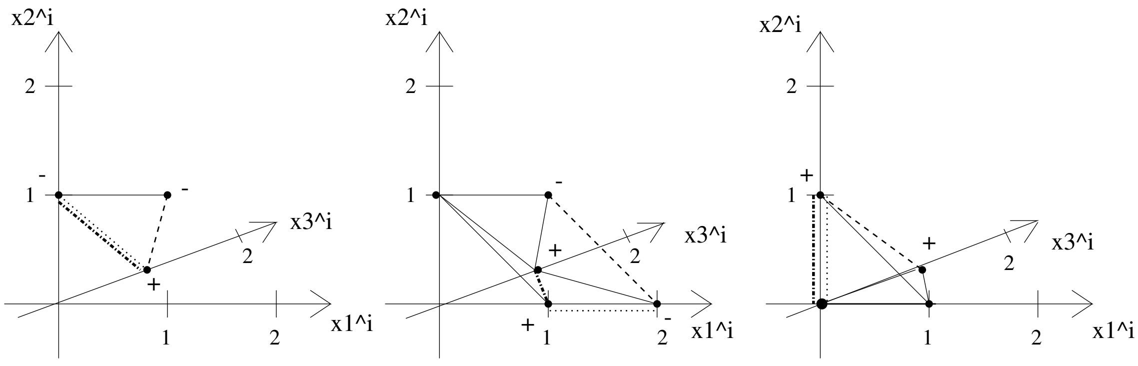

Figure 10: Mixed subdivision of Newton Polytopes of system by Edelstein.

The lifting

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

gives a mixed subdivision with three cells

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

as shown in Figure 10. 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 $(av_1 + im(YA)) \cap \mathbf{R}^3$. The alternating cell is part of the Newton polytopes which in turn are given by the directed graph and the bipartite graph. Figure 11 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 $1-3$ positive solutions.

The condition in Theorem 7.4 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 dominat 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 much larger than the rate constant of the associated backward reaction. We conclude that for chemical reaction systems Theorem 7.4 gives a realistic estimate for the number of positive solutions. The alternating cells as parts of the Newton polytopes correspond to

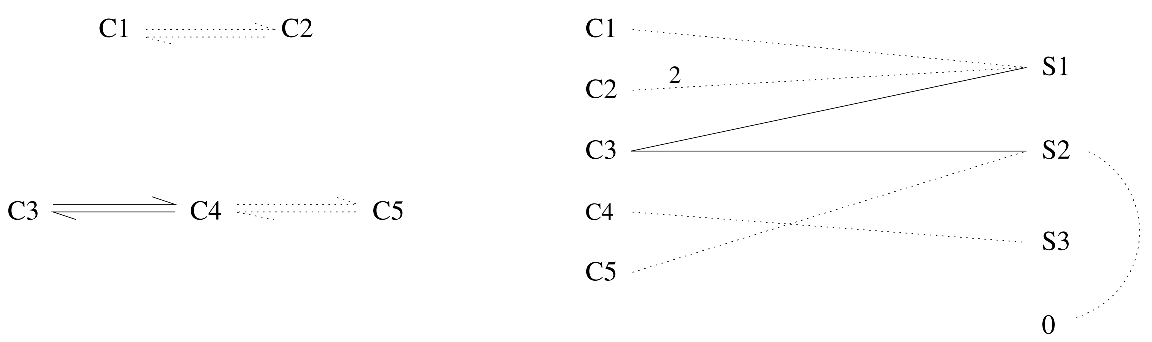

Figure 11: Parts of the directed graph of the example by Edelstein which corresponds to the alternating cell which is responsible for the positive solution.

parts of the directed graph. We conclude that we can identify parts of the directed graph or chemical reaction network which are responsible for positive solutions for some parameter region.

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Appendix

Proof of Theorem 3.4: The classification into connected components yields a decomposition $\mathbf{C}^n = L_1 \oplus \cdots \oplus L_l$ into invariant subspaces. Thus

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

Also T_ν^λ corresponding to terminal strong linkage classes are invariant. Thus

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

In order to show equality one needs to show that $A_{|R_\lambda}$ has full rank for all $\lambda = 1, \ldots, l$. This is equivalent to the following: if $v \in ker(A) \setminus \{0\}$ then $v_i = 0$ for all $i \in \bigcup_{\lambda=1}^{l} \mathcal{R}_\lambda$ corresponding to rests $\mathcal{R}_\lambda := \mathcal{L}_\lambda \setminus (\bigcup_\nu \mathcal{T}_\nu^\lambda)$. This is shown in three steps.

First we need to show that with $v \in ker(A)$ also $\tilde{v} \in ker(A)$ where $\tilde{v}_i := |v_i|$ for $i = 1, \ldots, n$. Recall

$$Av = \sum_{i=1}^{n} \sum_{y_j \to y_i \in R} k_{ij} v_j - \left(\sum_{y_i \to y_j \in R} k_{ij} \right) v_i = Kv - \mathrm{diag}(K^t e)v\,.$$

The components of Av are $(Av)_i = \sum_j k_{ij}v_j - \left(\sum_j k_{ji}\right) v_i$, $i = 1, \ldots, n$. This yields

$$v \in \ker(A) \quad \Rightarrow \quad \forall\, i \quad (Av)_i = 0 \quad \Rightarrow \quad \forall\, i \quad \left|\sum_{j=1}^{n} k_{ij}v_j\right| = \left|\left((\sum_{j=1}^{n} k_{ji}\right) v_i\right|.$$

Summation over all indices and the rules for norms give

$$\sum_{i=1}^{n}\sum_{j=1}^{n} k_{ij}|v_j| \geq \sum_{i=1}^{n}\left(\sum_{j=1}^{n} k_{ji}\right)|v_i|.$$

Since both sides are equal we must have

$$\sum_{j=1}^{n} k_{ij}|v_j| = \left(\sum_{j=1}^{n} k_{ji}\right)|v_i|, \quad i = 1, \ldots, n\,. \tag{15}$$

With $|v_i| = \tilde{v}_i$ this means $A\tilde{v} = 0$.

Secondly, if $v \in \ker(A)$ with $v_i = 0$ and $(C_j \to C_i) \in R$ then $v_j = 0$. This is an immediate consequence of $\sum_j k_{ij}|v_j| = (\sum_j k_{ji})|v_i|$ as in the previous part of the proof.

Consequently, if $C_j \to C_{\nu_1} \to C_{\nu_2} \to \cdots \to C_i$ and $v_i = 0$ then $v_j = 0$.

The third statement is that

$$v_i = 0, \quad \forall\; i \in \mathcal{R}_1 \cup \ldots \cup \mathcal{R}_l\,,$$

for all $v \in \ker(A)$. Since the connected components are invariant it suffices to consider one connected component $\mathcal{L}_\lambda$. Then the summation in (15) is over $j \in \mathcal{L}_\lambda$ only. Summation over $i \in \mathcal{T}_\lambda := \mathcal{T}_1^\lambda \cup \ldots \cup \mathcal{T}_{t_\lambda}^\lambda$ yields

$$\sum_{i\in\mathcal{T}_\lambda}\sum_{j\in\mathcal{L}_\lambda} k_{ij}|v_j| = \sum_{i\in\mathcal{T}_\lambda}\sum_{j\in\mathcal{L}_\lambda} k_{ji}|v_i|\,.$$

The sum in the left hand side is decomposed by $\mathcal{L}_\lambda = \mathcal{T}_\lambda \cup \mathcal{R}_\lambda$ and the right hand is simplified since $k_{ji} = k_{C_i \to C_j} = 0$ for $j \in \mathcal{R}_\lambda$ and $i \in \mathcal{T}_\lambda$ because members of terminal strong linkage classes do not react to the rest:

$$\sum_{i\in\mathcal{T}_\lambda}\sum_{j\in\mathcal{T}_\lambda} k_{ij}|v_j| + \sum_{i\in\mathcal{T}_\lambda}\sum_{j\in\mathcal{R}_\lambda} k_{ij}|v_j| = \sum_{i\in\mathcal{T}_\lambda}\sum_{j\in\mathcal{T}_\lambda} k_{ji}|v_i|\,.$$

Thus the second sum on the left is zero. This implies $v_j = 0$ for all $j \in \mathcal{R}_\lambda$ such that $C_j \to C_i$ for some $i \in \mathcal{T}_\lambda$. Since $\mathcal{L}_\lambda$ is a connected component all other $\mu \in \mathcal{R}_\lambda$ are strongly linked by some path $C_\mu \to \cdots \to C_j$. By the previous argument $v_j = 0$ implies $v_\mu = 0$. Altogether $v_i = 0$ for all $i \in \mathcal{R}_\lambda$. This means $\ker(A) \subseteq \bigoplus_\lambda \bigoplus_\nu T_\nu^\lambda$.

Since the T_ν^λ are invariant under A this yields the first statement

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

Obviously, $\ker(A) \cap T_\nu^\lambda \neq \{0\}$ since $\mathrm{im}(A_{|T_\nu^j})$ is generated by differences $\omega_i - \omega_j$.

The last statement $\dim(\ker(A) \cap T_\nu^\lambda) = 1$ is shown by contradiction.
Assume $\dim(\ker(A) \cap T_\nu^\lambda) \geq 2$ and let v and w be two linear independent vectors in $\ker(A) \cap T_\nu^\lambda$. Then there is a nontrivial linear combination $\alpha v + \beta w$ and $i \in \mathcal{T}_\nu^\lambda$ such that $(\alpha v + \beta w)_i = 0$. By the considerations above this implies $\alpha v + \beta w = 0$ which is a contradiction. $\square$

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