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Counting stable solutions of sparse polynomial systems in chemistry

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ABSTRACT. The polynomial differential system modeling the behavior of a chemical reaction is given by graph theoretic structures. The concepts from toric geometry are applied to study the steady states and stable steady states. Deformed toric varieties give some insight and enable graph theoretic interpretations. The importance of the circuits in the directed graph are emphasized. The counting of positive solutions of a sparse polynomial system by B. Sturmfels is generalized to the counting of stable positive solutions in case of a polynomial differential equation. The generalization is based on a method by sparse resultants to detect whether a system may have a Hopf bifurcation. Special examples from chemistry are used to illustrate the theoretical results.

1. Introduction

In chemistry a class of polynomial differential equations arise which has a lot of discrete structure in the coefficients and the monomials:

$$\dot{x} = Y_s I_a I_K \Psi(x), \quad \Psi(x) = \begin{pmatrix} x^{\eta_1} \\ \vdots \\ x^{\eta_n} \end{pmatrix},$$

is given by adjacency matrices and incidence matrices of two weighted graphs. A detailed description of the problem is given in Section 2. One is interested in the positive steady states, stable ones and Hopf points, especially depending on the structure of the graphs and for all positive values of the involved constants k_{ij} . This fascinating problem shows a very rich mathematical structure and several mathematical disciplines may be applied.

Numerical methods are not suitable since several (too many) unknown constants are involved and one is interested in global statements while numerical investigations are local.

There are several known results. Especially, the early work in [C180] has influenced a lot the chemical literature like [EBSE96, E94, HS98]. The papers [F, F95a, F95b] (for explanation see also [GH99]) include special interesting results for a special subclass ($Y_s = Y_k$). In [MMN89] symbolic computation has been

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applied to such chemical systems for the first time. They applied Gröbner bases as a black box neglecting the structure of the problem. Of course Gröbner bases are very important for the study of positive solutions ([GRRT99]), but in this problem class the computation of a Gröbner bases of the given polynomials ignore the graph theoretic structures. That's why the use of Gröbner bases is restricted to study toric ideals which appear.

Toric varieties turn out to be very useful if they are adjusted to this particular application. The generalization is even suitable for the study of positive solutions. A realistic example illustrates this principle and nicely interpreted by substructures of the graphs.

But the main result is the counting of stable positive solutions by a generalization of ideas from [St94, St98]. For this reason the new polynomial $Res_{B,H}$ is introduced. The vanishing of $Res_{B,H}$ is a necessary condition that a dynamical system has a Hopf point.

The structure of the paper is as follows. Section 2 describes the given data and the structure of the differential equations precisely. Deformed toric varieties and graph theoretic investigation of a convex polyhedral cone are the topics of Section 3 while Section 4 investigates Hopf bifurcation with resultants and bialternate products. Finally, Section 5 gives the main result of this paper, the counting of positive stable steady states as a generalization of the counting of positive solutions in [St94, St98].

2. Mass action kinetics - a sparse polynomial system

An interesting system of ordinary differential equations consisting of sparse polynomials is defined by two graphs as presented in [GH99].

The first graph is a *weighted bipartite graph*. The two sets of vertices consist of $S_i, i = 1, \dots, m$ and $C_j, j = 1, \dots, n$. To each edge $\{S_i C_j\}$ there are two weights $y_{ij} \in \mathbf{N}$ and $\eta_{ij} \in \mathbf{N}$ associated. This defines two weighted adjacency matrices whose relevant parts are $Y_s = (y_{ij})_{i=1, \dots, m, j=1, \dots, n}$ and $Y_k = (\eta_{ij})_{i=1, \dots, m, j=1, \dots, n}$. We denote the columns of Y_s by $y_1, \dots, y_n \in (\mathbf{Z}_{\geq 0})^m$ and the columns of Y_k by $\eta_1, \dots, \eta_n \in (\mathbf{Z}_{\geq 0})^m$. We assume that Y_s and Y_k have the same support (i.e. $y_{ij} = 0$ iff $\eta_{ij} = 0$ and $y_{ij} > 0$ iff $\eta_{ij} > 0$) and that $\eta_{ij} \leq y_{ij}, \forall i = 1, \dots, m, j = 1, \dots, n$. Moreover, we assume that $y_i \neq y_j$ or $\eta_i \neq \eta_j$ for all $i \neq j$. Additionally, we assume that every vertex S_i is adjacent at least to one vertex C_j . But there may be C_j without incident edges.

Secondly, there is a *weighted directed graph* with vertices $C_i, i = 1, \dots, n$ and oriented edges $C_j \rightarrow C_i$ for some $i, j \in \{1, \dots, n\}$. Each oriented edge (arrow) $C_j \rightarrow C_i$ from reactant C_j to product C_i has a weight $k_{C_j \rightarrow C_i} = k_{ij} \in \mathbf{R}_+$. This information is encoded in the weighted adjacency matrix $K = (k_{ij}) \in (\mathbf{R}_{\geq 0})^{n,n}$ with $k_{ij} = 0$ if $C_j \rightarrow C_i$ is not an arrow. We assume that for each vertex C_i there is at least one adjacent edge. An oriented edge $C_j \rightarrow C_i$ and its opposite $C_i \rightarrow C_j$ with two different associated constants are simultaneously possible. But there are no parallel edges.

Beside the adjacency matrix the directed graph has two incidence matrices. The first incidence matrix is $I_a = (w_{ij})_{i=1, \dots, n, j=1, \dots, l}$ where $w_{ij} \in \{-1, 0, 1\}$ and a denotes the number of arrows. Each column represents an oriented edge by containing one entry -1 for the reactant and 1 for the product. The second incidence matrix is $I_K = (u_{\mu\nu})_{\mu=1, \dots, l, \nu=1, \dots, n}$ with $u_{\mu\nu} \in \{k_{ij} \mid i, j = 1, \dots, n\}$ or $u_{\mu\nu} = 0$.

TABLE 1. The algebra-chemistry dictionary.

SNA <u>stoichiometric network analysis</u>	
Y_s stoichiometric matrix	$A = I_a I_K$ kinetic matrix
$S = \text{im}(Y_s I_a)$ stoichiometric space	$\text{im}(Y_s I_a I_K) = \text{im}(Y_s A)$ kinetic space
$v_i \perp \text{im}(Y_s A)$ conservation vector ($v_i \geq 0$)	$\exists v_i \perp \text{im}(Y_s A), v_i > 0$ conservative
$v_i^t x - a_i$ conservation relations ($v_i \geq 0$)	$\delta = \text{rank}(I_a) - \text{rank}(Y_s I_a)$ deficiency
$A\Psi(x)$ complex formation vector	$Y_s A\Psi(x)$ species formation vector
$I_K\Psi(x)$ reaction velocity vector	
k_{ij} rate constant	K rate constant matrix
y_{ij} stoichiometric coeff. or molecularity	η_{ij} kinetic exponent
C_i complexes	S_i chemical species
reaction $C_j \rightarrow C_i$ with reactant complex C_j and product complex C_i	
$S_i \rightarrow 2S_i$ autocatalytic reaction	
minimal generator E_i of cone $\ker(Y_s I_a) \cap (\mathbf{R}_{\geq 0})^l$ extreme current	

Each row corresponds to one oriented edge and has at most one non-zero entry. The μ -th arrow $C_j \rightarrow C_i$ gives $u_{\mu j} = k_{ij}$ encoding the weight and that C_j is the reactant complex.

Altogether, this defines the following polynomial differential equation

$$(2.1) \quad \dot{x} = Y_s A\Psi(x), \quad \text{with} \quad \Psi(x) = \begin{pmatrix} x^{\eta_1} \\ \vdots \\ x^{\eta_n} \end{pmatrix},$$

where $A = I_a I_K = K - \text{diag}(K^t e)$ and $x = (x_1, \dots, x_m) \in (\mathbf{R}_{\geq 0})^m$.

In [C180] the matrix $\underline{\nu} := Y_s I_a$ is used. With $v(x) = I_K\Psi(x)$ system (2.1) is written as

$$(2.2) \quad \dot{x} = \underline{\nu} v(x).$$

Moreover, $v(x)$ may be written as $D\chi(x)$ with a diagonal matrix $D \in (\mathbf{R}_{\geq 0})^{l,l}$ containing diagonal entries $d_{\mu,\mu} = k_{ij}$ for the μ -th arrow $C_j \rightarrow C_i$ and a vector of monomials $\chi(x) = (x^{\kappa_1}, \dots, x^{\kappa_l})^t$, $\chi_\mu(x) = x^{\eta_j}$. The matrix κ of exponents as used in [C180] is formed from the columns of Y_k . More precisely they are formed from the columns of Y_r which is given by those columns η_i from Y_k for which an arrow $C_i \rightarrow C_j$ exists.

A special case is that Y_s can be chosen such that $Y_s = Y_k$. Then system (2.1) is a stoichiometric system or with *mass action kinetics*¹. This name stems from the fact that the graphs naturally arise in chemistry where (2.1) describes the evolution of the concentrations x_i of the chemical species S_i . Also all other quantities have a special name as summarized in Table 1.

System (2.1) has flow-invariant subspaces of the form $(x_0 + \text{im}(Y_s A)) \cap (\mathbf{R}_{\geq 0})^m$, see Lemma 2.7 in [GH99]. Thus one restricts the investigation of steady states to those satisfying

$$v_i^t x - a_i = 0, \quad i = 1, \dots, m - \text{rank}(Y_s A),$$

¹The precise definition of mass action kinetics is that it is not pathological ($\exists \nu_{ij} < 0, \kappa_{ij} = 0$) and for each pair of forward reaction i and backward reaction j we have $\nu_i = \kappa_j - \kappa_i$, where $\nu_i, \kappa_j, \kappa_i$ are columns of the matrices $\underline{\nu}$ and κ .

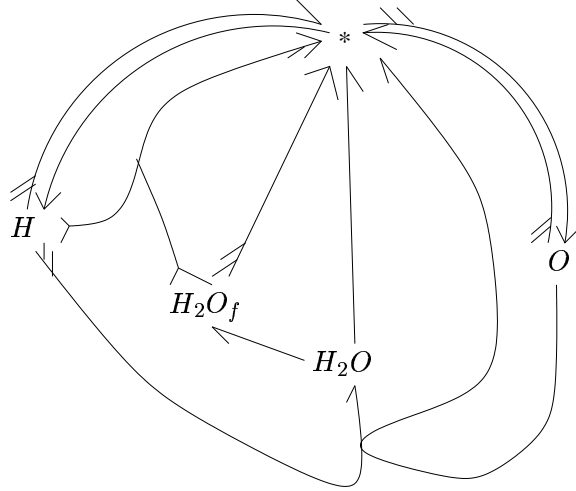


FIGURE 1. Field emitter tip: H_2/O_2 reaction on the tip of a thin metal within an electric field as presented in [EBSE96]. The number of barbs gives y_{ij} within a reactant complex and the total number of feathers gives y_{ij} within a product complex while the number of feathers to the left gives η_{ij} . The vacant ads-space on the tip of the metal is symbolized by $*$.

where v_i form an orthonormal basis of the orthogonal complement of $\text{im}(Y_s A)$ and the $a_i \in \mathbf{R}$ are given constants. In the literature often $\text{im}(Y_s I_a)$ is used. But in case a connected component includes several terminal strong connected components then $\text{rank}(I_a I_K) < \text{rank}(I_a)$. If $\text{rank}(Y_s A) < \text{rank}(Y_s I_a)$ the v_i depend on the constants k_{ij} in general.

Even more one is interested in *stable* points (i.e. real parts of all eigenvalues of Jacobian negative) and *Hopf points* (eigenvalues $\pm i\omega$). Since $\text{im}(Y_s A)$ is flow-invariant the notions of stability and Hopf points are modified in Section 4.

The graph theoretic definitions are explained by the following typical example which was taken from [EBSE96].

EXAMPLE 2.1. Figure 1 and Figure 2 show the same information on a chemical reaction in an analogous way.

The differential equations are

$$\begin{aligned}
 \dot{x}_1 &= -k_{2,1}x_1x_2^2 - 2k_{10,7}x_1^2 + 2k_{7,10}x_5^2 \\
 \dot{x}_2 &= -2k_{2,1}x_1x_2^2 - 2k_{9,3}x_2^2 - 2k_{11,8}x_2x_4 + 2k_{3,9}x_5 \\
 \dot{x}_3 &= k_{2,1}x_1x_2^2 + (-k_{5,4} - k_{9,4})x_3 \\
 \dot{x}_4 &= k_{5,4}x_3 - 2k_{10,6}x_4^2 - 2k_{11,8}x_2x_4 \\
 \dot{x}_5 &= k_{2,1}x_1x_2^2 + k_{9,3}x_2^2 + k_{9,4}x_3 + 2k_{10,6}x_4^2 + 2k_{10,7}x_1^2 + 3k_{11,8}x_2x_4 \\
 &\quad - k_{3,9}x_5 - 2k_{7,10}x_5^2
 \end{aligned}$$

where x_1, \dots, x_5 are the concentrations of O, H, H_2O , H_2O_f and the amount of space on the metal, respectively.

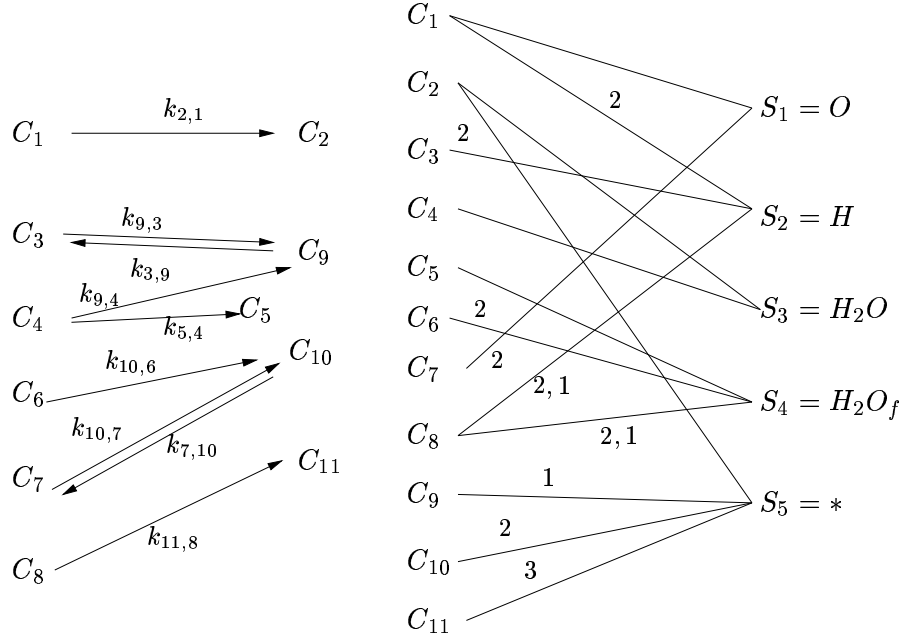


FIGURE 2. Information from Figure 1 as a weighted directed graph and a weighted bipartite graph. An edge in the bipartite graph without number has weights $y_{ij} = \eta_{ij} = 1$. If one number is associated to the edge then $y_{ij} = \eta_{ij}$ else $y_{ij} > \eta_{ij}$.

We have $\text{rank}(I_a I_K) = 6$, $\text{rank}(I_a) = 7$, $\text{rank}(Y_s I_a I_K) = \text{rank}(Y_s I_a) = 4 < 5 = m$. The additional linear restriction is given by

$$v_1^t x - a_1 = \begin{pmatrix} 2 & 1 & 2 & 2 & 2 \end{pmatrix} x - a_1 = 0.$$

◇

The nice thing about system (2.1) is that almost all mathematical terms have a graph theoretic meaning. For example we may consider the combined graph from the directed graph and the bipartite graph since the vertices C_i appear in both. If the combined graph has several connected components then system (2.1) decouples.

In [FH77] it is explained how the structure of the directed graph determines by connected components, strong connected components and *terminal strong connected components* the structure and the rank of the matrix $A = I_a I_K$. This knowledge is exploited in the work [F], [F95a], [F95b]. An explanation of this is given in [GH99].

3. Deformed toric varieties and positive steady states

This section is started with the discussion of complex solutions $x \in (\mathbf{C} \setminus \{0\})^m$ of $Y_s A \Psi(x) = 0$ with the help of toric varieties. If one neglects the property of normality they are defined as $X_{\hat{Y}_k} = V(I_{\hat{Y}_k}) = \{z \in \mathbf{C}^n \mid f(z) = 0 \forall f \in I_{\hat{Y}_k}\}$ $I_{\hat{Y}_k} = \{f \in \mathbf{C}[z_1, \dots, z_n] \mid f(x_0 x^{n_1}, \dots, x_0 x^{n_n}) \equiv 0\}$. Binomial generators of $I_{\hat{Y}_k}$ are computed by the usual implicitation of varieties with Gröbner bases or more

efficiently by Algorithms 12.3 and 12.6 in [St96]. See also [KM99] for efficient computation with ideals of this type.

The advantages of toric varieties are well-known. The degree of the toric variety (computed by the coefficient of the Hilbert polynomial [St96] p. 36 or by the mixed volume of the Newton polytopes by mixed subdivision [CLO98]) gives the number of toric solutions for generic coefficients since $I_{\hat{Y}_k}$ does not depend on the coefficients. The facets of the Newton polytopes are used to explain when for special values of the coefficients some solutions $x \in (\mathbf{C} \setminus \{0\})^m$ escape to points with components zero or to infinity ([CLO98] p. 309).

For positive real solutions one needs to discuss the intersection of the convex polyhedral cone $\ker(Y_s A) \cap (\mathbf{R}_{\geq 0})^n$ (of dimension $n - \text{rank}(Y_s A)$) with $X_{\hat{Y}_k}$ which is the basis of the deficiency-one-theorem [F95a] as explained in [GH99]. Once a generating vector z of an intersection line is known $z = x_0 \Psi(x)$ is solved by Hermite normal form.

In this application one can take advantage of the special structure. The first obvious property is that not all monomials appear. Remember that the columns of Y_r are formed by those η_i for which an arrow $C_i \rightarrow C_j$ exists. Then one would consider the homogeneous toric ideal $I_{\hat{Y}_r}$. But one can even better take advantage of the structure. Because the coefficient matrix in our application is a product of Y_s , I_a and I_K and all constants are positive a variant of this principle has even more advantages. We use

$$I_{\hat{K}} = \{f \in \mathbf{C}(\underline{k})[z_1, \dots, z_l] \mid f(x_0 v_1(x), \dots, x_0 v_l(x)) \equiv 0\},$$

where \underline{k} collects all appearing non-zero k_{ij} , and its variety $V(I_{\hat{K}})$ and the convex polyhedral cone $\ker(Y_s I_a) \cap (\mathbf{R}_{\geq 0})^l$. The advantage in comparison to the standard approach is that the cone does not involve the constants k_{ij} . We denote the elements of a minimal set of generators by E_i .

LEMMA 3.1. (i) *If $\text{rank}(Y_s I_a) = \text{rank}(I_a)$ then the positive circuits of the directed graph generate the convex polyhedral cone $\ker(Y_s I_a) \cap (\mathbf{R}_{\geq 0})^l$. Then the minimal generators E_i are given by those positive circuits which are not a convex combination of other positive circuits.*

(ii) *Let the set of indices $\{1, \dots, l\}$ decompose with respect to the connected components L_λ and even further decompose with respect to terminal strong connected components $L_\lambda = T_\lambda^\nu \cup \dots \cup T_\lambda^{t_\lambda} \cup R_\lambda$. Define $I_\lambda^\nu = (w_{ij})_{i=1, \dots, n, j \in T_\lambda^\nu}$ where $I_a = (w_{ij})_{i=1, \dots, n, j=1, \dots, l}$. If $\text{rank}(Y_s I_\lambda^\nu) = \text{rank}(I_\lambda^\nu)$ then the positive circuits of the terminal strong connected components (λ, ν) which are not convex combinations of other positive circuits define minimal generators E_i .*

While the positive circuits are oriented cycles in the directed graph the other minimal generators have an interpretation in the combined graph consisting of the directed graphs without weights k_{ij} and the bipartite graph with weights y_{ij} , see the example below. Note that the cone is not necessarily simplicial, although in many practical situations this will be the case because $\text{rank}(I_a) - \text{rank}(Y_s I_a)$ is small and $\ker(I_a) \cap (\mathbf{R}_{\geq 0})^l$ is a simplicial cone if the directed graph is not complicated.

The generators E_i may be computed by the simplex algorithm from linear programming. But here no linear functional is optimized. A variant of the simplex algorithm is used to enumerate all vertex vectors. Of course one likes to take advantage of the graph theoretic information within this computation. Since $Y_s I_a$ is integer there is even a relation to Gröbner bases. Algorithm 4.5 in [St96] may be

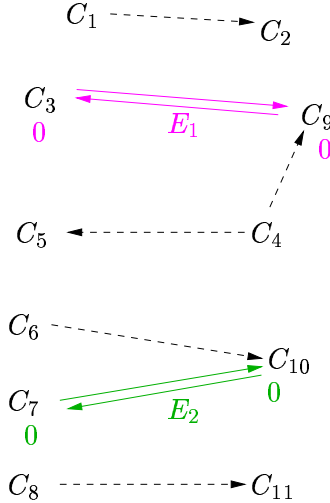


FIGURE 3. Minimal generators E_1 and E_2 of the convex polyhedral cone which are positive circuits in the directed graph.

used and an universal Gröbner basis may be computed which by Proposition 4.11 in [St96] includes all circuits. The circuits of type $z^E - 1$ will give our minimal generators. The computation of an universal Gröbner basis (equivalently the determination of the Gröbner fan and the state polytope) works for toric ideals efficiently even for larger problems as shown in [TH99].

Because of the importance of the cone $\ker(Y_s I_a) \cap (\mathbf{R}_{\geq 0})^l$ the computation of a minimal set of generators E_i is studied a lot in the chemical literature ([C180], [HS98] and references therein). There the fact is used that each $z \in \ker(Y_s I_a) \cap (\mathbf{R}_+)^l$ gives a positive solution $x \in \mathbf{R}^m$ if the k_{ij} are chosen appropriately. On the other hand if the constants k_{ij} are given the vector $z \in \ker(Y_s I_a) \cap (\mathbf{R}_{\geq 0})^l$ has to satisfy the condition $z \in V(I_{\hat{\kappa}})$.

LEMMA 3.2. (i) The ideal $I_{\hat{\kappa}}$ in $\mathbf{C}(\underline{k})[z]$ is generated by binomials in $\mathbf{Q}[\underline{k}][z]$. (ii) Each vertex C_i in the directed graph which is incident to two (or more) oriented edges pointing out from C_i gives one (or several) linear polynomial(s) in $I_{\hat{\kappa}}$. (iii) $I_{\hat{\kappa}}$ and $I_{\hat{\gamma}_r}$ have the same Hilbert series and the same Hilbert polynomial.

PROOF. (i) $I_{\hat{\kappa}}$ is clearly generated by binomials because a Gröbner basis of the elimination ideal $I_{\hat{\kappa}} = \langle \{z_i - x_0 v_i(x) \mid i = 1, \dots, l\} \rangle \cap \mathbf{Q}(\underline{k})[z]$ may be computed by the Buchberger algorithm where all involved polynomials are binomial if the input polynomials are binomial. (ii) Two arrows $C_i \xrightarrow{\alpha} C_j$ and $C_i \xrightarrow{\beta} C_\nu$ give $v_\alpha = k_{ji} x^{n_i}$, $v_\beta = k_{\nu i} x^{n_i}$ and thus $k_{\nu i} z_\alpha - k_{j i} z_\beta$. (iii) The Hilbert series and the Hilbert polynomial are build from the vector space dimensions of $(\mathbf{C}[z_1 \dots, z_n]/I_{\hat{\gamma}_r})_d$ and $(\mathbf{C}[z_1 \dots, z_l]/I_{\hat{\kappa}})_d$ of degrees $d \in \mathbf{N}$. But for each additional variable in z_1, \dots, z_l there is a linear polynomial by (ii) such that the dimensions are equal. \square

Each binomial in $I_{\hat{\kappa}}$ has an interpretation in the combined graph formed from the directed graph with weights k_{ij} and the bipartite graph with weights η_{ij} , see the example below.

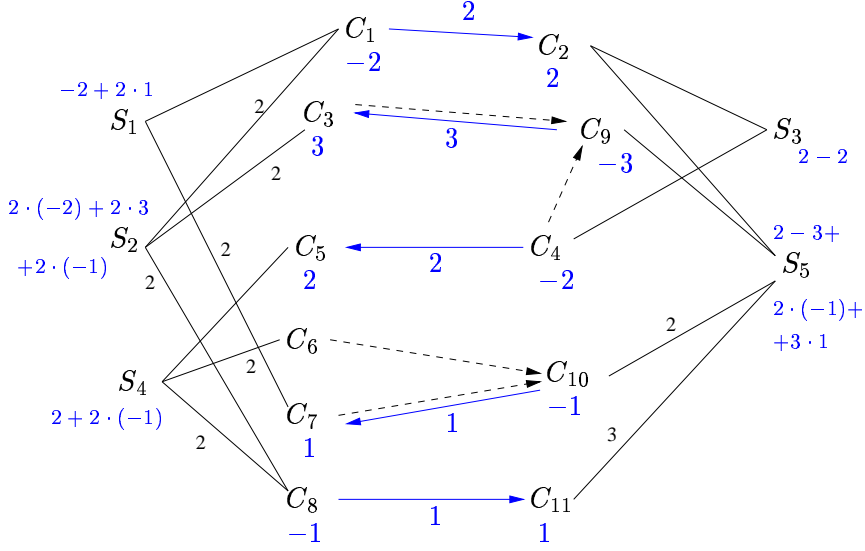


FIGURE 4. Minimal generator E_3 of the cone. The numbers associated to the arrows are $E_3 = [2, 0, 3, 0, 2, 0, 0, 1, 1]$ while the weights on the vertices C_i are given by the entries of $I_a E_3 = [-2, 2, 3, -2, 2, 0, 1, -1, -3, -1, 1]$. The computations associated to the vertices S_i stand for $Y_s(I_a E_3)$.

Geometrically, the variation of values of all $k_{ij} > 0$ means that the variety $V(I_{\hat{k}})$ just deforms without changing basic properties. The variety $V(I_{\hat{Y}_r})$ is clearly isomorphic to $V(I_{\hat{k}})$ in case all $k_{ij} = 1$ since for additional variables z_i we have linear equations $z_i = z_{j(i)}$. Thus for all positive choices of k_{ij} the varieties $V(I_{\hat{k}})$ and $V(I_{\hat{Y}_r})$ are isomorphic. While $X_{\hat{Y}_k}$ contains the orbit $O_1 = \{z \in (\mathbf{C} \setminus \{0\})^n \mid \exists t_0, \dots, t_m \text{ with } z = (t_0 \prod_{i=1}^m t_i^{\eta_{i1}}, \dots, t_0 \prod_{i=1}^m t_i^{\eta_{in}})\}$ as an open and dense set the deformed toric variety $V(I_{\hat{k}})$ contains the orbit $O_{I_K \mathbf{1}} = \{z \in (\mathbf{C} \setminus \{0\})^l \mid \exists t_0, \dots, t_m \text{ with } z = \text{diag}(t_0 \prod_{i=1}^m t_i^{\kappa_{i1}}, \dots, t_0 \prod_{i=1}^m t_i^{\kappa_{in}}) I_K \mathbf{1}\}$ as a dense and open set. Even more the structure of subvarieties corresponding to points at infinity or with zero-components is the same. That means that the property that toric solutions escape to infinity depends on the structure of the graphs, but *not* on their weights. It seems that the positive circuits in the directed graph often turn out to be important in this context.

EXAMPLE 3.3. (Example 2.1 continued) A minimal set of generators of the convex polyhedral cone $\ker(Y_s I_a) \cap (\mathbf{R}_{\geq 0})^l$ is found by elementary linear algebra

$$\begin{aligned} E_1 &= [0, 1, 1, 0, 0, 0, 0, 0, 0] & E_2 &= [0, 0, 0, 0, 0, 0, 1, 1, 0] \\ E_3 &= [2, 0, 3, 0, 2, 0, 0, 1, 1] \\ E_4 &= [2, 0, 2, 0, 2, 1, 0, 1, 0] \\ E_5 &= [2, 0, 2, 2, 0, 0, 0, 1, 0]. \end{aligned}$$

While $I_a E_1 = I_a E_2 = 0$ because these two are positive circuits in the directed graph (see Figure 3) the other three are interpreted in the combined graph as

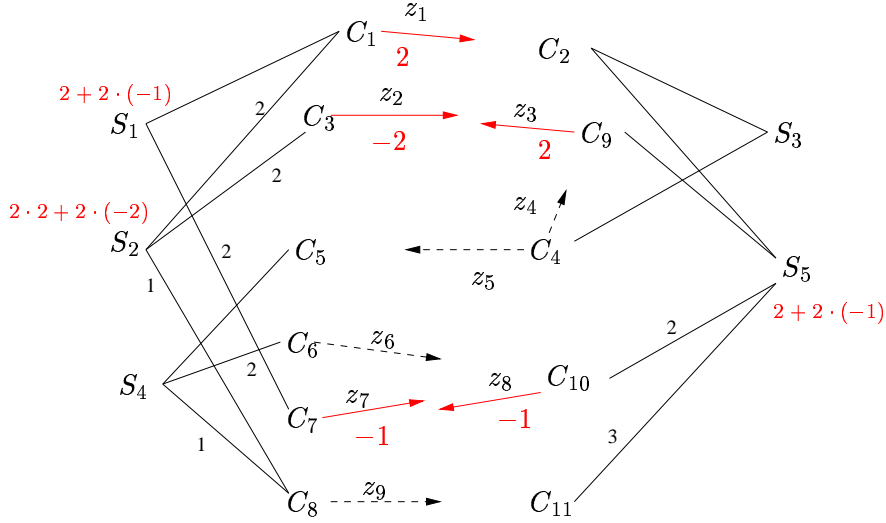


FIGURE 5. The exponents of the 3. binomial $z_1^2 z_3^2 - c(\underline{k}) z_2^2 z_8 z_7$ correspond to a vector in the kernel of κ which corresponds to a kernel vector of $Y_{\underline{k}}$.

illustrated in Figure 4 for E_3 . A Gröbner basis of the deformed toric ideal is computed by using

$$\begin{aligned} z_1 &= k_{2,1} \hat{x}_1 \hat{x}_2^2 \hat{x}_0 & z_2 &= k_{9,3} \hat{x}_2^2 \hat{x}_0 & z_3 &= k_{3,9} \hat{x}_5 \hat{x}_0 \\ z_4 &= k_{9,4} \hat{x}_3 \hat{x}_0 & z_5 &= k_{5,4} \hat{x}_3 \hat{x}_0 & z_6 &= k_{10,6} \hat{x}_4^2 \hat{x}_0 \\ z_7 &= k_{10,7} \hat{x}_1^2 \hat{x}_0 & z_8 &= k_{7,10} \hat{x}_5^2 \hat{x}_0 & z_9 &= k_{11,8} \hat{x}_2 \hat{x}_4 \hat{x}_0 \end{aligned}$$

giving

$$-k_{5,4} z_4 + k_{9,4} z_5, \quad k_{11,8}^2 z_6 z_2 - k_{9,3} k_{10,6} z_9^2, \quad k_{10,7} k_{9,3}^2 k_{7,10} z_1^2 z_3^2 - k_{3,9}^2 k_{2,1}^2 z_2^2 z_8 z_7.$$

Substituting $\sum_{i=1}^5 \lambda_i E_i$ gives three polynomials in λ

$$\begin{aligned} &-2 k_{5,4} \lambda_5 + k_{9,4} (2 \lambda_3 + 2 \lambda_4), \quad k_{11,8}^2 \lambda_4 \lambda_1 - k_{9,3} k_{10,6} \lambda_3^2, \\ &k_{10,7} k_{9,3}^2 k_{7,10} (2 \lambda_3 + 2 \lambda_4 + 2 \lambda_5)^2 (\lambda_1 + 3 \lambda_3 + 2 \lambda_4 + 2 \lambda_5)^2 \\ &\quad - k_{3,9}^2 k_{2,1}^2 \lambda_1^2 (\lambda_2 + \lambda_3 + \lambda_4 + \lambda_5) \lambda_2. \end{aligned}$$

CASE $\lambda_3 = 0$: Then case $\lambda_1 = 0$ gives $\lambda_4 = \lambda_5 = 0$ and λ_2 arbitrary. The case $\lambda_4 = 0$ leads to $\lambda_5 = 0$ and $\lambda_1 = 0$ and λ_2 arbitrary or opposite $\lambda_2 = 0$ and λ_1 arbitrary.

CASE $\lambda_3 \neq 0$: Because we work in homogeneous coordinates we may choose $\lambda_3 = 1$ and receive from the first two equations

$$\lambda_5 = \frac{k_{9,4} (k_{11,8}^2 \lambda_1 + k_{9,3} k_{10,6})}{k_{11,8}^2 \lambda_1 k_{5,4}}, \quad \lambda_4 = \frac{k_{9,3} k_{10,6}}{k_{11,8}^2 \lambda_1}.$$

Substitution into the third gives one polynomial in λ_1, λ_2

$$c_2(\underline{k}) \lambda_1^6 \lambda_2^2 + (c_{16}(\underline{k}) \lambda_1^6 + c_{15}(\underline{k}) \lambda_1^5) \lambda_2 - c_{00}(\underline{k}) - \cdots - c_{06}(\underline{k}) \lambda_1^6$$

which is quadratic in λ_2 having positive coefficients of λ_2^2 and λ_2 and negative constant $c_0(\lambda_1, \underline{k})$ if we consider λ_1 to be positive. There is *one* family of positive

solutions parameterized by $\lambda_1 \geq 0$. For given λ_2 there may be at most two values of λ_1 by Descartes' rule of signs.

The limits are of particular interest. Since points with zero-components or at infinity correspond to facets we investigated the 8 facets of the 5-dimensional polytope $\text{conv}(\eta_1, \eta_3, \eta_4, \eta_6, \eta_7, \eta_8, \eta_9, \eta_{10})$. Not all facets allow for non-negative real points. One facet corresponds to $\lambda_5 = 0$ while another corresponds to $\lambda_3 = \lambda_4 = 0$. Neighboring facets allow for real points only for $\lambda_1 E_1$ or $\lambda_2 E_2$. Since the real part of the variety is homeomorphic to the polytope ([F93] p. 81) the curve parameterized by λ_1 is homeomorphic to a curve within the 5-dimensional polytope. It connects two facets which are further investigated with the momentum map which projects a point on the toric variety to a convex combination of the vertices of the polytope. If $\lambda_1 \rightarrow \infty$ then $\lambda_2 \rightarrow c_2(\underline{k})$, $\lambda_4 \rightarrow 0$, $\lambda_5 \rightarrow c_5(\underline{k})$. The limit of the image of the momentum map approaches $k_{3,9}/(k_{3,9} + k_{9,3})\kappa_2 + k_{9,3}/(k_{3,9} + k_{9,3})\kappa_3$ which corresponds to E_1 . Then $x \rightarrow (0, 0, 0, 0, 0)$. If $\lambda_1 \rightarrow 0$ then $\lambda_2 \rightarrow \infty$ like $1/\lambda_1^3$ and $\lambda_4 \rightarrow \infty$, $\lambda_5 \rightarrow \infty$ the image of the momentum map goes to $k_{7,10}/(k_{7,10} + k_{10,7})\kappa_7 + k_{10,7}/(k_{7,10} + k_{10,7})\kappa_8$ which corresponds to E_2 . Then x tends to infinity.

For arbitrary λ_1 we may solve for x_i (\hat{x}_i) in $I_K \Psi(\hat{x})\hat{x}_0 = z$ in terms of roots by Hermite normal form. This transforms the linear equation to

$$2 \frac{w_1^3}{w_2^4 w_5^2} + \frac{w_1^3}{w_5^3 w_2^4} + 2 \frac{w_3 w_1^4}{w_5^4 w_2^6} + 2 \frac{w_4 w_1^3}{w_5^3 w_2^4} + 2 \frac{w_6 w_1^4}{w_5^4 w_2^6} - a_1 = 0,$$

where $w_i = w_i(\underline{k}, \lambda_1)$, $i = 1, 2, 3, 4, 6$ and $w_5 = c_5(\underline{k}) \cdot \frac{\sqrt{\lambda_2}}{\sqrt{\lambda_1}}$. Of course λ_1, λ_2 still need to satisfy the equation above from the toric ideal. Depending on the value of $a_1 > 0$ one expects several positive solutions. \diamond

An alternative way includes the linear conditions right from the beginning. Then

$$\begin{pmatrix} Y_s J_a & \mathbf{0} & & \\ & v_1^t & a_1 & \\ & \vdots & \vdots & \\ \mathbf{0} & v_r^t & a_r & \end{pmatrix} \begin{pmatrix} v(x) \\ x_1 \\ \vdots \\ x_m \\ 1 \end{pmatrix} = B\chi(x) = 0.$$

has the coefficient matrix B and monomial vector χ . The minimal set of generators of the convex polyhedral cone $\ker(B) \cap (\mathbf{R}_{\geq})^{a+m+1}$ are partially known as $(E_i^t, 0)$ from the set of minimal generators of $\ker(Y_s J_a) \cap (\mathbf{R}_{\geq 0})^l$. Unfortunately, in general v_i will involve the constants k_{ij} as already a_i are entering the computation of the cone. Moreover, the discussion will be complicated and depend on the values of a_i for vectors v_i which are non-negative for conservative systems, but in general are not. The computation of the generators of the toric ideal is done analogously and substitution of a convex combination of the generators of the cone gives equations in λ .

EXAMPLE 3.4. (Example 2.1 and 3.3 continued)

Lifting $\eta_1, \eta_3, \eta_4, \eta_6, \eta_7, \eta_8, \eta_9, \eta_{10}, e_1, e_2, e_3, e_4, e_5, 0$ and computing a Gröbner basis of the toric ideal with Maple gives the Hilbert polynomial

$$\frac{1}{5} \lambda^5 + \frac{13}{12} \lambda^4 + \frac{8}{3} \lambda^3 + \frac{47}{12} \lambda^2 + \frac{47}{15} \lambda + 1,$$

with degree 24 which means that the system has for generic values of coefficients at most 24 complex solutions and thus at most 24 real positive solutions.

For completeness we mention that one might as well work with Minkowski summands of the Newton polytopes, either by forming the sum of the two obvious summands or more tricky by distinguishing several Newton polytopes after linear manipulation of $Y_s A \Psi(x)$. This leads to higher dimensional convex polyhedral cones and toric ideals in rings with many variables. This may turn out to be inefficient.

4. Finding Hopf bifurcation with resultants

The aim of the next section is the generalization of the method of counting positive solutions valid for some parameter regions as explained in [St94] and [St98]. In this section we will give some necessary definitions from dynamical systems and prepare the generalization.

A dynamical system is given by $\dot{x} = f(x)$ where $f : \mathbf{R}^n \rightarrow \mathbf{R}^n$ is a C^∞ -function. A steady state $x_0 \in \mathbf{R}^n$ is called *stable*, if all eigenvalues of the Jacobian $D_x f(x_0) \in \mathbf{R}^{n,n}$ have negative real part. We consider a system $\dot{x} = f(x, \lambda)$ where $f : \mathbf{R}^{n+1} \rightarrow \mathbf{R}^n$ depends on an additional parameter and like to know how the stable steady states depend on λ . Assume a C^∞ -branch $(x(s), \lambda(s))$ of steady state solutions then the eigenvalues of $D_x f(x(s), \lambda(s))$ depend C^∞ on the parameter s . Starting with a stable point $x_0 = x(s_0)$ the real parts of the eigenvalues have two possibilities to turn positive. Either a real eigenvalue crosses 0 (in a bifurcation point) or a pair of complex eigenvalues crosses the imaginary axis. The last situation is called *Hopf bifurcation* because the pair of eigenvalues $\pm i\omega$ together with some genericity conditions guarantee the bifurcation of a branch of *periodic solutions* (oscillations). A good reference is [GH83] p. 151.

Criteria are known to decide numerically when a real matrix C (which is a Jacobian $D_x f(x_0, \lambda_0) \in \mathbf{R}^{n,n}$) has a pair of complex eigenvalues $\pm i\omega$. These methods use algebraic concepts.

The first method uses resultants and works efficiently for $n < 10$. From the characteristic polynomial $p(\mu) = \det(\mu Id - C)$ one constructs two polynomials $q_e(\mu^2) = p(\mu) + p(-\mu)$ and $q_o(\mu^2) = (p(\mu) - p(-\mu))/\mu$ of degree $\lfloor n/2 \rfloor$. Since $q_e(-\omega^2) = q_o(-\omega^2) = 0$ it follows for the Sylvester resultant $Res(D_x f) = Res(q_e, q_o, \mu) = 0$ if the matrix C has a pair of eigenvalues $\pm i\omega$. This method has been successfully applied numerically in the program LocBif.

The second method uses the bialternate product of matrices (see e.g. [Go00] p. 94). This associates to C a matrix $2C \odot Id$ of dimension $\frac{n(n-1)}{2}$

$$(2C \odot Id)_{(i,j),(k,l)} = \begin{cases} -a_{il} & \text{if } k = j \\ a_{ik} & \text{if } k \neq i \text{ and } l = j \\ a_{ii} + a_{jj} & \text{if } k = i \text{ and } l = j \\ a_{jl} & \text{if } k = i \text{ and } l \neq j \\ -a_{jk} & \text{if } l = i \\ 0 & \text{else.} \end{cases}$$

The index pairs satisfy $i > j$ and $k > l$. If C has eigenvalues $\pm i\omega$ then $2C \odot Id$ has eigenvalue zero. Thus $p_\odot = \det(2C \odot Id) = 0$ is a necessary condition for a dynamical system to have a Hopf point. This is used in the program Content.

These methods may be applied in order to check whether a system $\dot{x} = f(x, \lambda)$ where f is polynomial in x and λ over a field F may have a Hopf bifurcation at all.

LEMMA 4.1. *Let $f(x, \lambda; \underline{k}) \in (F[\underline{k}][x, \lambda])^n$ be a polynomial vector where F is an appropriate field. Let $Res(D_x f(x, \lambda; \underline{k}))$, $p_\odot \in F[\underline{k}][x, \lambda]$ be the polynomials constructed above. If the system $\dot{x} = f(x, \lambda; \underline{k})$ has for some fixed values \underline{k}_0 a Hopf point at (x_0, λ_0) then $Res(x_0, \lambda_0, \underline{k}_0) = 0 = p_\odot(x_0, \lambda_0, \underline{k}_0)$. If (x_0, λ_0) is a bifurcation point then $\det(D_x f(x_0, \lambda_0, \underline{k}_0)) = 0$. If x_0 is positive then the toric Jacobian $\det(\text{diag}((x_0)_1, \dots, (x_0)_n) D_x f(x_0, \lambda_0, \underline{k}_0))$ has eigenvalue zero.*

Since a bifurcation point satisfies $n + 1$ sparse polynomial equations in n variables x_1, \dots, x_n the sparse resultant ([CLO98] Sec. 7.2) may be applied. Then $Res_{B,T}(\lambda_0, \underline{k}_0) = 0$ where B denotes the support of f as polynomials in x and T the support of the determinant of the toric Jacobian. This was used in [St98]. In analogy one may check for Hopf points by the sparse resultant $Res_{B,H}(\lambda_0, \underline{k}_0)$ where H is the support of $Res(D_x f)$ or of p_\odot as a polynomial in x . For problems of moderate size it is possible to construct (multiples) of these sparse resultants ([EC95, EM99]).

For system (2.1) $f(x; \underline{k}) = Y_s I_a I_K \Psi(x)$ is clearly polynomial, but the situation is slightly different. Since affine shifts of $\text{im}(Y_s A)$ are flow-invariant a steady state x_0 is called to *stable within* $x_0 + \text{im}(Y_s A)$ if the restricted Jacobian has the property that all eigenvalues have negative real part. Analogously, Hopf points within $x_0 + \text{im}(Y_s A)$ are defined. Thus we use an orthonormal basis of $\text{im}(Y_s A)$ and form a matrix $U \in F^{m,s}$ from these vectors where s is the dimension of $\text{im}(Y_s A)$. Then $C = U^t Y_s I_a I_K D_x \Psi(x) U$ is a polynomial matrix in $F[x, \underline{k}]^{s,s}$. Then the resultant from the first method and the determinant of the bialternate product are polynomials in $F[x, \underline{k}]$. We consider it as a polynomial in $F[\underline{k}][x]$, as well as $U^t Y_s I_a I_K \Psi(x)$ as s polynomials. The linear equations $v_i^t x - a_i$, $i = 1, \dots, m - s$ are polynomials in $F[\underline{k}, \underline{a}][x]$. Then the sparse resultant is a polynomial in $F[\underline{k}, \underline{a}]$. If system (2.1) undergoes some Hopf bifurcation for some value of some parameter $\lambda = k_{ij}$ (and where the remaining k_{ij} are constant) then the sparse resultant vanishes for these values.

EXAMPLE 4.2. (Example 2.1 simplified) We simplify the H_2O example such that no H_2O_f is involved ($x_4 = 0$). Then we compute $Res(x, \underline{k})$ and $p_\odot(x, \underline{k})$ explicitly in Maple. They turn out to be different. Unfortunately, the formulas are so complicated that no information can be extracted.

This example shows that in general this treatment of Hopf bifurcation is not efficient. Concepts in numerics and in symbolic computation are so different that methods from numerics can not be transferred without rethinking. Nevertheless the polynomials $Res(x, \underline{k})$ and $p_\odot(x, \underline{k})$ are important for theory and thus are used in the next section.

In [C180] it is suggested to use the minimal generators E_i of the convex polyhedral cone and the Routh-Hurwitz theorem to determine the stability of all steady states. This requires further research and a careful investigation with methods from algebraic geometry and analysis.

5. The number of stable solutions

In the beginning of this section we consider the general polynomial situation:

$$\dot{x} = f(x; \underline{c}), \quad \text{where } f_{ij} = \sum_{b \in B_i} c_b^j x^b, \quad i = 1, \dots, r, j = 1, \dots, k_i$$

with $k_1 + \dots + k_r = n$ and supports $B_i \subset (\mathbf{Z}_{\geq 0})^n$.

The theory in [HS95, St94, St98] is based on a special homotopy which enables to divide the polynomial system into binomial systems which are easily solved. This is

$$H_{ij}(x, t) = \sum_{b \in B_i} c_b^j x^b t^{\omega_i(b)},$$

where the integer values $\omega_i(b)$ are chosen randomly. Geometrically, the Newton polytopes are lifted and the lower hull of the lifted polytopes gives a mixed subdivision of the Newton polytopes for generic lifting values. Moreover, generically one may assume that the mixed cells are even simple mixed.

DEFINITION 5.1. ([HS95], [VG95])

(i) A *subdivision* of $B = (B_1, \dots, B_r)$ is a collection $S = \{C_1, \dots, C_s\}$ of s cells $C_j = (C_j^{(1)}, \dots, C_j^{(r)})$ such that

- (a) $\dim(\text{conv}(C_j)) = n$ for $j = 1, \dots, s$,
- (b) $\text{conv}(C_j) \cap \text{conv}(C_k)$ is a common face of $\text{conv}(C_j)$ and of $\text{conv}(C_k)$ for all pairs $C_j, C_k \in S$,
- (c) $\bigcup_{j=1}^s \text{conv}(C_j) = \text{conv}(B)$.

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

- (d) $\sum_{\lambda=1}^r \dim(\text{conv}(C_j^{(\lambda)})) = n$ for all cells $C_j \in S$ holds.

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

- (e) $\dim(\text{conv}(C_j^{(\lambda)})) = k_\lambda, \quad \lambda = 1, \dots, r$.

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

- (f) $\sum_{\lambda=1}^r (\#(C_j^{(\lambda)}) - 1) = n$

holds.

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

The idea is that each mixed cell gives a small subsystem of the original system $f(x; \underline{c}) = 0$ corresponding to a facet of the lower hull. Along the homotopy this generically continues to solutions of $f(x; \underline{c}) = 0$. Additionally, one may check the stability for $t = 0$. If no bifurcation or Hopf bifurcation occurs along the homotopy then the number of stable, positive solutions at $t = 0$ equals the number of stable, positive solutions at $t = 1$, i.e. for the original system $f(x, \underline{c}) = 0$.

Motivated by the signed Newton polytopes a mixed cell of the subdivision is called *alternating* in [IR96], if the associated binomial system has precisely one positive solution.

THEOREM 5.2. Consider f, H as above with generic lifting values $\omega_i(b) \in \mathbf{Z}$. Assume that the induced mixed subdivision is simple mixed and that the coefficients \underline{c} are such that the following conditions are satisfied.

- (i) The sparse resultant $\text{Res}_{B, T}(\underline{c}, \underline{a}, t)$ has no zero for $t \in (0, 1]$.
- (ii) None of the small systems associated to a facet has infinitely many solutions.
- (iii) The sparse resultant $\text{Res}_{B, H}(\underline{c}, \underline{a}, t)$ has no zero for $t \in (0, 1]$.

Then the number of stable positive solutions is the same for $t = 0$ and $t = 1$.

PROOF. The proof of Bernstein's theorem in [HS95] is based on Puiseux expansions

$$x(t) = \begin{pmatrix} u_1 t^{\gamma_1} \\ \vdots \\ u_n t^{\gamma_n} \end{pmatrix} + \text{higher order terms in } t,$$

where $(\gamma, 1)$ is an inner normal to one of the facets of the lower hull of the lifted Newton polytopes. The complex solutions of the associated binomial system are candidates for u . By Hensel's lemma they give rise to a Puiseux expansion. In [St94, St98] it was observed that $x(t)$ is real and positive for all $t \in (0, \varepsilon)$ with ε sufficiently small iff u is real and positive. This argumentation uses the coordinate transformation $x_i = u_i t^{\gamma_i}$, $i = 1, \dots, n$ and

$$g_{ij}(u, t) = \frac{1}{t^{m_i}} H_{ij}(ut^\gamma, t) = \sum_{b \in C^{(i)}} c_b^j x^b + \text{hot in } t, \quad j = 1, \dots, k_i, \quad i = 1, \dots, r,$$

where $C = (C^{(1)}, \dots, C^{(r)})$ is a simple mixed cell defined by the facet of the lower hull and m_i is the minimal value of the linear functional defined by $(\gamma, 1)$ on the lifted Newton polytope. A positive solution $(u, 0)$ gives by the theorem of implicit functions a branch of positive solutions $(u(t), t)$ for t small which yields a branch of positive solutions $(x(t), t)$.

By the first two conditions it is guaranteed that the homotopy paths stay positive, finite and do not undergo a bifurcation. Then the number of positive solutions of $f(x; \underline{c}) = 0$ equals the number of alternating cells.

According stability we observe that generically $D_u g(u, 0)$ is regular and thus one may decide on stability. Suppose all eigenvalues have negative real part. Since the eigenvalues depend C^∞ on the parameter t the points $(u(t), t)$ are stable for $\dot{u} = g(u, t)$ for sufficiently small t . The Jacobian matrices are related as

$$\text{diag}\left(\frac{1}{t^{m_i}}\right) D_x H(x(t), t) \text{diag}(t^{\gamma_k}) = D_u g(u(t), t).$$

Multiplication with positive diagonal matrices from both sides does not change the signs of the real parts of the eigenvalues. This implies stability of $(x(t), t)$ for small t . One may use the equivalent characterization of stability

$$\xi^t B J \xi < -\delta x^t J \xi \quad \forall \xi \in \mathbf{R}^n,$$

where J is the Jacobian, $\delta > 0$ a constant, and B a symmetric positive definite matrix. With this criterion the desired conclusion is easily observed.

By the third condition there is no Hopf bifurcation along the homotopy. Thus the number of alternating cells whose positive solution is stable equals the number of stable steady states of $\dot{x} = f(x; \underline{c})$. \square

In the chemical reaction system (2.1) the situation is slightly different since there are flow-invariant subspaces. But a modified version is still valid.

THEOREM 5.3. *Assume a chemical reaction system*

$$\dot{x} = Y_s I_a I_K \Psi(x), \quad \Psi(x) = \begin{pmatrix} x^{\eta_1} \\ \vdots \\ x^{\eta_n} \end{pmatrix},$$

defined by a weighted bipartite graph and a weighted directed graph together with the conservation relations $v_i^t x - a_i$, $i = 1, \dots, m - \text{rank}(Y_s I_a I_K)$. Assume that the

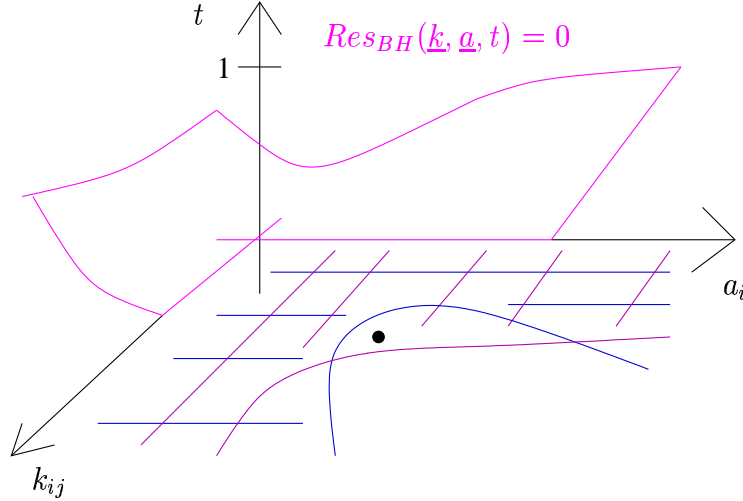


FIGURE 6. Schematic picture for Theorem 5.3. The set $\{(\underline{k}, \underline{a}) \mid \exists t \in (0, 1), Res_{BT}(\underline{k}, \underline{a}, t) = 0\}$ is shown for which a system f with the constants $(\underline{k}, \underline{a})$ admits a bifurcation along the homotopy. Analogously, $\{(\underline{k}, \underline{a}, t) \mid t \in (0, 1), Res_{BH}(\underline{k}, \underline{a}, t) = 0\}$ is shown and its projection $\{(\underline{k}, \underline{a}) \mid \exists t \in (0, 1), Res_{BH}(\underline{k}, \underline{a}, t) = 0\}$. The point symbolizes a system f where the associated homotopy might have a Hopf point, but no bifurcations, see Figure 7.

lifting values of the two supports $B_1 = \{\eta_i \mid \eta_i \text{ column in } Y_r\}$ and the m -simplex $B_2 = \{0, e_1, \dots, e_m\}$ are chosen such that the mixed subdivision is simple. The lifting values define a homotopy

$$H_1(x, t; \underline{k}) = Y_s I_a I_K \begin{pmatrix} x^{\eta_1} t^{\omega_1(\eta_1)} \\ \vdots \\ x^{\eta_n} t^{\omega_1(\eta_n)} \end{pmatrix}$$

$$H_{2j}(x, t; \underline{a}) = (x_1 t^{\omega_2(e_1)}, \dots, x_m t^{\omega_2(e_m)}) v_j - a_j t^{\omega_2(0)},$$

where $j = 1, \dots, m - \text{rank}(Y_s A)$. Assume the constants $k_{ij} \in \mathbf{R}_+$ and parameter a_i are chosen such that the following conditions are satisfied along the homotopy.

- (i) The sparse resultant $Res_{B,T}(\underline{k}, \underline{a}, t)$ has no zero for $t \in (0, 1]$.
- (ii) None of the small systems associated to a facet has infinitely many solutions.
- (iii) The sparse resultant $Res_{B,H}(\underline{k}, \underline{a}, t)$ has no zero for $t \in (0, 1]$. This sparse resultant is constructed from the equations $Y_s I_a I_K \Psi(x) t^{\omega_1} = 0$, the conservation relations $v_j^t x t^{\omega_2} - a_j t^{\omega_2(0)} = 0$ and the determinant of the bialternate product of the Jacobian matrix $U^t Y_s I_a I_K D_x \Psi(x) t^{\omega_1} U$, where the columns of U form an orthonormal basis of $\text{im}(Y_s I_a I_K)$.

Then the number of stable positive points of $Y_s I_a I_K \Psi(x) = 0$ within a subspace $x_0 + \text{im}(Y_s A) \cap (\mathbf{R}_+)^m$ equals the number of stable positive points of the binomial systems.

Of course it will be difficult to compute the sparse resultants as polynomials in $\underline{k}, \underline{a}$, but for given values $\underline{k}_0, \underline{a}_0$ one might evaluate its value numerically.

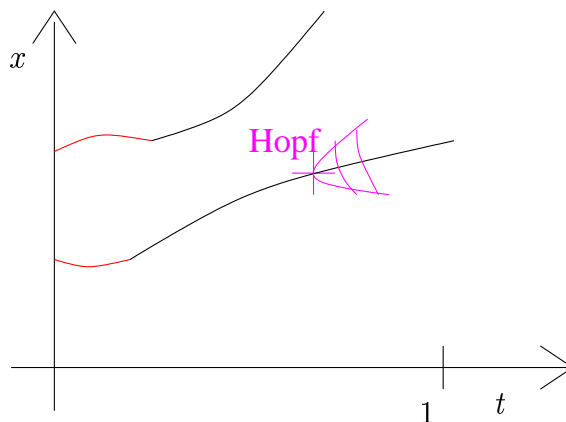


FIGURE 7. The homotopy for a system corresponding to the point in Figure 6. There may be a Hopf point, but no bifurcation points.

A mixed cell $(C^{(1)}, C^{(2)})$ of the supports have graph theoretic meaning. It corresponds to a subgraph of the combined graph.

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