Using Distance to Bifurcation to Quantify the Resilience of Nonnegative Dynamical Systems

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***Abstract*— This paper describes the use of sums-of-square (SOS) program to compute a resilience measure for non-negative dynamical systems. Such measure is defined as the distance between system's nominal parameter and the closest critical paramater at which a bifurcation occur. Our proposed method uses a modeling formalism from chemical reaction network theory to describe the dynamics of nonnegative system. We show that such modeling formalism allow us to describe the bifurcation condition only in term of system's parameter. The SOS program for computing the distance to the closest bifurcation is formulated using the positvstellensatz concept from real algebraic geometry and the SOS relaxation technique in semidefinite programming.**

I. INTRODUCTION

Many real life systems are subject to external perturbations which cause variation on systems parameters from the nominal values. For nonlinear systems, parameter variation of certain magnitude can change the qualitative behaviors of the system (i.e. phase portrait or stability) through a bifurcation. A bifurcation is characterized by the appearance of a *topologically nonequivalent* phase portrait of the system [1]. In many cases, these changes come with catastrophic effects. For example, load variation in power network which exceeds certain treshold can induces a saddle node bifurcation that causes a voltage collapse [2], [3]. Another example is in the lake eutrophication process where the increase of nutrient loading which exceeds a critical limit results in a saddle node bifurcation that shifts a previously clear water lake with high biodiversity into a turbid water lake dominated by algae [4]. Each of these effects has the potential to disrupt the services that these systems provide to the society. Understanding the resilience of these systems in the presence of parameter variation is therefore crucial for managing their security and sustainability [5], [6].

The resilience of a system under parameter variation can be measured by the distance $\gamma = |k^* - k^0|$ between the nominal parameter k^0 and the closest critical paramater k^* at which a bifurcation occur. The quantity γ, often called *distance to closest bifurcation*, is an indication of how close the system is to a collapse. The computation of γ is generally difficult since the *bifurcation set* in the parameter space that contain μ^* is usually unknown. For dynamical systems

$$\dot{x} = f(x, k), \tag{1}$$

whose equilibrium x^* depend on parameter k, the bifurcation set are those parameters k that satisfy the bifurcation conditions in table I. Previous works have proposed several methods for computing γ in the context of robust stability analysis [7], [8], [9], [10] and voltage collapse in power systems [2], [3]. In general, these methods use numerical optimization techniques to search for the minimum γ subject to the constraints that the critical parameter k^* satisfy the bifurcation condition in table I. These methods, however, are computationally demanding since the search for minimum γ requires the computation of equilibrium x^* at every iteration.

TABLE I: Local bifurcation condition

Type	Jacobian Eigenvalue	Transversality
Hopf	simple 0	$D_k\{Re(s)\} \neq 0$
Saddle node	simple imaginary pair	$w\left(D_k f\big\|_{x^*,k^*}\right) \neq 0$ $w\left(D_x^2 f\big\|_{(v,v)}\right) \neq 0$
Transcritical	simple imaginary pair	$w\left(D_k f\big\|_{x^*,k^*}\right) \neq 0$ $w\left(D_{x,k}^2 f\big\|_{v,v}\right) \neq 0$
Pitchfork	simple imaginary pair	$w\left(D_k f\big\|_{x^*,k^*}\right) \neq 0$ $w\left(D_x^3 f\big\|_{x^*,k^*}\right) \neq 0$

This paper uses sums-of-square (SOS) programming method to compute the resilience measure γ of non-negative dynamical systems. Our method stems from recognizing that non-negative dynamical systems (1) have a special structure (see equation (2)) that allow us to compute an analytical parameterization of the equilibrium in term of the system parameter. The method for this equilibrium parameterization was first introduced in the context of stoichiometric network analysis and is based on the concept of *toric variety* from algebraic geometry [11]. Such parameterization is beneficial for computing γ since we can now express the constraint functions only in term of the parameters. We formulate the optimization of γ as an SOS program using the positivstellensatz concept from real algebraic geometry [12], [13] and the SOS relaxation technique in semidefinite programming [14]. The optimal γ obtained from the SOS program is a lower bound of some positive semidefinite function $V(\mu)$ and is guaranteed to be a global minimum with respect to a prespecified parameterization of $V(\mu)$. The SOS program can be solved efficiently using SOSTOOLS [15] and semidefinite program solver such as Sedumi [16].

The remainder of the paper is structured as follows.

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Section II describes the model structure. Section III discusses semialgebraic description for bifurcation condition in table I. Section IV presents the characterization of bifurcation-free parameter set and SOS program to compute the minimum γ. Section V illustrates an application of the proposed method to study the resilience of a tritrophic food chain from ecology.

Notational convention: Let $\mathbb{R}, \mathbb{Q}$ and $\mathbb{Z}$ denote the set of real, rational and integer numbers, respectively, and let $\mathbb{R}_+$ and $\mathbb{Z}_+$ the set of non-negative real and non-negative integer numbers, respectively. Let $\mathbb{R}^n$ denote the n-dimensional Euclidean vector space. Given a vector $x \in \mathbb{R}^n$, we let x_i denote the ith component of that vector. An n-dimensional *multi-index* is an n-tuple, $\alpha \equiv (\alpha_1, \alpha_2, \cdots, \alpha_n)$ of non-negative integers. The absolute value of a multi-index α is defined as $|\alpha| = \sum_{i=1}^n \alpha_i$. The sum/difference of two multi-indices in $\mathbb{Z}_+^n$ is the component wise sum/difference of the indices. Similarly, we say that $\alpha \geq \beta$ if and only if $\alpha_i \geq \beta_i$ for $i = 1, 2, \ldots, n$.

Given a vector $x \in \mathbb{R}^n$ and an n-dimensional multi-index α, a *monomial* in x with total degree $|\alpha|$ is a product of the form $x^\alpha \equiv x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n}$. A monomial ordering is used to arrange a pair of monomials unambiguously in an ascending/descending order. Let $\alpha = (\alpha_1, \ldots, \alpha_n)$ and $\beta = (\beta_1, \ldots, \beta_n)$ be multi-indices of vector $x \in \mathbb{R}^n$. We say α and β is in lexicographic (lex) ordering $\alpha >_{lex} \beta$ if the left-most nonzero entry of the vector $\alpha - \beta$ is positive. A lex ordering of monomials $x^\alpha >_{lex} x^\beta$ is satisfied if $\alpha >_{lex} \beta$. Let $\mathbb{F}$ be any field such as the real numbers ($\mathbb{F} = \mathbb{R}$) . A pth order polynomial in n unknown $x = (x_1, \ldots, x_n)$ with coefficients $k = (k_1, \ldots, k_p)$ in the field $\mathbb{F}$ is a finite linear combination of monomials of the form

$$f(x, k) = \sum_{|\alpha| \leq p} k_\alpha x^\alpha, \text{ with } k_\alpha \in \mathbb{F}.$$

The set of all such polynomials form a *polynomial ring* denoted by $\mathbb{F}(k)[x]$. We mostly consider polynomial ring over the real field. For $i = 1, \ldots, q$, the solution to polynomial equations $f_i(x, k) = 0$ with $f_i \in \mathbb{R}(k)[x]$ is the set of all its zeros, i.e. the set $\{x \in \mathbb{Q}^n(k) : f_i(x, k) = 0\}$. A polynomial $f(x, k)$ is said to be *nonnegative* or *positive semidefinite* (psd) if $f(x, k) \geq 0, \forall x \in \mathbb{R}^n$. A necessary condition for a polynomial to be psd is that its total degree is even.

Definition 1.1: We say that the polynomial $f(x, k)$ is SOS if it can be rewritten as $f(x, k) = \sum_{i=1}^s q_i^2(x, k)$ for some polynomials $q_i(x, k), i = 1, \ldots, s$.

Clearly, a polynomial $f(x, k)$ being SOS implies $f(x, k)$ is psd. We use $\mathcal{P}_n^{2d}$ to denote the set of SOS polynomials in n unknowns with degree less than or equal to $2d$.

II. System Model

Consider dynamical system described as follows.

$$\begin{aligned} \dot{x}(t) &= f(x, k), \text{ with } f(x, k) \in \mathbb{R}(k)[x] \\ &= Nv(x, k), \end{aligned} \tag{2}$$

where $x \in \mathbb{R}_+^n$ is the state vector, $k \in \mathbb{R}_+^p$ is the parameter vector, $N \in \mathbb{Z}^{n \times m}$ is a sparse matrix, and $v(x, k) \in \mathbb{R}_+^m$ is a *rate* vector consisting monomials in the unknown x with real coefficient k. The rate vector can be decomposed as $v(x, k) = \text{diag}(k)x^Z$, with $Z \in \mathbb{Z}_+^{n \times m}$ is a matrix whose ith column is the multi-index of the ith monomials in $v(x, k)$. If matrix N has no full row rank (i.e. $rank(N^T) = r < n$), there exist conservation relations of the form $W^T x = c$, where $W \in \mathbb{Z}^{(n-r) \times m}$ is a matrix whose column form the basis of $ker(N^T)$ and c is an appropriately dimensioned constant vector. Equation (2) is often used in stoichiometric network analysis (SNA) to model the dynamics of chemical species x that involved in a reaction of rate $v(x, k)$ [17].

This paper uses the structure in (2) to model non-negative dynamical systems in (1). System (1) is said to be nonnegative if $x(t) \in \mathbb{R}_+^n$ for all $t \in [0, \infty)$. The necessary condition for system (1) to be non-negative is that for all $k \in \mathbb{R}_+^p$, it satisfy $f(x, k) \geq 0$ when $x \in \mathbb{R}_+^n$ and $f(x, k) = 0$ otherwise. Non-negative dynamical systems cover a large number of real world systems including compartmental systems, biological systems, ecological systems, etc [18]. In general, the model of these systems does not always satisfies the conditions in model (2), i.e. the vector field $f(x, k)$ being polynomial functions defined over polynomial ring $\mathbb{R}(k)[x]$. The well-known result from approximation theory [19], however, states that any analytic functions defined over a compact set can always be approximated as closely as desirable by polynomial function. Moreover, there are also exist techniques for transforming any rational polynomial functions into polynomial functions defined over polynomial ring [20]. These facts show that model (2) can cover a large class of non-negative dynamical systems and therefore the parameterization of their equilibrium set and Jacobian matrix can also be obtained using the techniques discussed above.

The zeros of (2) define the *state equilibrium* x^*

$$x^* = \{x \in \mathbb{Q}^n(k) : Nv(x, k) = 0\}, \tag{3}$$

such that x^* is a vector in $\mathbb{R}^n$ for fixed k, and is a continuum otherwise. Computating the analytical expression for equilibrium (3) in high dimensional systems usually requires the use of symbolic methods. One of such methods is based on the techniques from algebraic geometry which uses the Gröbner basis of equations $Nv(x, k) = 0$ [21]. This method originates from the fact that the zeros of polynomial equations are equivalent with the zeros of its basis. Gröbner bases of polynomial equation can be computed using Buchberger algorithm which have been implemented in many computer algebra softwares [22]. The standard Buchberger algorithm, however, has a drawback in that (in the worst case) the degree of the computed bases grow doubly exponential with respect to the number of unknown variables [23].

An alternative method to characterize x^* is proposed in [11], [24] by taking advantage from the structure of (2) in which $f(x, k)$ is decomposed into linear (N) and nonlinear ($v(x, k)$) parts. Such decomposition define an isomorphic mapping $v(x, k)$ from the state x to the rate v of the form

$$v(x, k) : \mathbb{R}[x] \mapsto \mathbb{R}[v], \quad x \mapsto v = kx^Z. \tag{4}$$

This isomorphism implies that the state equilibrium x^* can

be characterized if the *rate equilibrium* v^* in (5) is known.

$$v^* = \{v \in \mathbb{Q}^m(k,\lambda) : Nv = 0\}, \tag{5}$$

where λ is known as *convex parameter*. In particular, the rate equilibrium v^* is parameterized by the intersection of two geometric objects namely *toric variety* and *convex polyhedral cone*. Both of these objects can be computed efficiently using techniques from algebraic geometry and convex analysis [11], [24]. On one hand, the toric variety provides a parameterization of the rate equilibrium, $v^*(k)$, in term of system parameters (k). It can be obtained from the Gröbner bases of the kernel of (4) using a modified Buchberger algorithm (more efficient with worst case complexity only exponential) [25]. On the other hand, one can observe from (5) that the rate equilibrium v^* is confined to the set $\mathcal{K}_v = \{ker(N) \cap \mathbb{R}^m_+\}$. The set $\mathcal{K}_v$ is a convex polyhedral cone and gives another parameterization $v^*(\lambda)$ in term of some convex parameter λ. The intersection of these two geometric objects forms a reparameterization of the rate equilibrium, $v^*(\lambda,k)$, in term of parameters (λ,k). By the isomorphic mapping in (4), the state equilibrium parameterization $x^*(\lambda,k)$ that correspond to a given $v^*(\lambda,k)$ can be obtained using Hermite transformation (see appendix B and [26] for details).

An implication of such parameterization is that the Jacobian matrix (Jac) of (2) at equilibrium is given by [11], [24]

$$Jac(\lambda,k) = N\text{diag}(v^*)Z^T\text{diag}(1/x^*). \tag{6}$$

This implies that the bifurcation condition in table I can be evaluated directly in term of the parameter (λ,k) without having to compute the equilibrium x^* for different k.

III. Semialgebraic Condition for Bifurcation

Consider dynamical systems in (2) and assume that its equilibrium x^* is asymptotically stable for an initial parameter k^0. When the parameter vary from its initial value k^0, then x^* and the phase portrait of the system will also vary in the state space. If such parameter variation crosses a certain treshold k^*, the equilibrium x^* may lose stability in bifurcation. A bifurcation is characterized by the appearance of new phase portrait (at $k = k^*$) around the equilibrium x^* that is *topologically nonequivalent* with the original one (at $k = k^0$) [1]. Since the phase change that being considered is locally around the equilibrium, this type of bifurcation is called local bifurcation. There are different types of local bifurcation which correspond to different changes of the phase portrait including *hopf* (appearance of limit cycle from stable equilibrium), *saddle node* (collision and annihilation of two equilibria), *pitchfork* (appearance or dissapearance of symmetric equilibria), and *transcritical* (stability change).

The appearance of local bifurcation is related with the change on the number or stability of the equilibriums under parameter variation. Thus, these changes can be characterized in term of the *eigenvalue condition* of the Jacobian matrix with some additional *transversality conditions* (see table I). The critical parameter k^* at which bifurcation occur is usually searched numerically using continuation method [1]. This method, however, is currently limited to low dimensional parameter space ($p \leq 3$). The main reason for such limitation is because the evalution of bifurcation condition in table I requires the knowledge of system's equilibrium x^* which is difficult to obtain in practice. The parameterized Jacobian matrix Jac in (6), however, is defined at equilibrium and so the eigenvalue condition in table I can be analyzed without having to compute the equilibrium x^* for all possible parameter k. This section presents semialgebraic descriptions of bifurcation condition in table I.

Consider the Jacobian matrix (6). Let $p(s) = |sI - Jac|$ be the characteristic polynomial of Jac defined as

$$p(s) = a_0 s^n + a_1 s^{n-1} + \cdots + a_{n-1}s + a_n, \tag{7}$$

where the coefficients $a_i(\lambda,k)$ are function of the parameters (λ,k). Towards the end, we denote these parameters as $\mu = (\lambda,k)$. The eigenvalues of Jac is given by the roots of $p(s)$, and matrix Jac is asymptotically stable if and only if all its eigenvalues have negative real parts and it is unstable otherwise. For $z = 1,\ldots,n$, the zth Hurwitz determinant, $\triangle_z$, associated with the characteristic polynomial $p(s)$ is

$$\triangle_z = \begin{vmatrix} a_1 & a_3 & a_5 & \cdots & a_{2z-1} \\ a_0 & a_2 & a_4 & \cdots & a_{2z-2} \\ 0 & a_1 & a_3 & \cdots & \cdots \\ \vdots & \vdots & \vdots & \ddots & a_{z+1} \\ 0 & 0 & 0 & a_{z-2} & a_z \end{vmatrix}$$

such that

$$\triangle_1 = |a_1|, \triangle_2 = \begin{vmatrix} a_1 & a_3 \\ a_0 & a_2 \end{vmatrix}, \triangle_3 = \begin{vmatrix} a_1 & a_3 & a_5 \\ a_0 & a_2 & a_4 \\ 0 & a_1 & a_3 \end{vmatrix}, \ldots$$

The coefficients a_i's and Hurwitz determinant $\triangle_z$'s can be used to infer some properties about the roots of $p(s)$ [27] . For example, the *Routh Hurwitz criterion* states that all roots of $p(s)$ will have negative real parts if and only if $a_n > 0$ and $\triangle_z > 0$ for $z = 1,\ldots,n$. The *Orlando formula* gives the relationship between the $(n-1)$th Hurwitz determinant and the roots of $p(s)$ of the form

$$\triangle_{n-1} = (-1)^{n(n-1)/2} a_0^{n-1} \prod_{i<j}^{1,\ldots,n} (s_i + s_j), \quad \text{for } n \geq 2.$$

The following propositions give the conditions for matrix Jac to have simple zero eigenvalue.

Proposition 3.1: Consider matrix Jac in (6) with characteristic polynomial $p(s)$ in (7). If $p(s)$ satisfies the conditions $a_n = 0$ and $a_{n-1} \neq 0$, then matrix Jac will have zero eigenvalue with multiplicity not greater than one.

Proof: That $a_n = 0$ implies one of the roots of $p(s)$ is zero is clear. Now notice that $p(s)$ will have zero eigenvalue with multiplicity not greater than one if

$$\frac{\partial p(s)}{\partial s}\Big|_{s=0} \neq 0,$$

which will be satisfied when $a_{n-1} \neq 0$. ■

The following lemma from [28] gives the condition for Jac to have a simple pair of imaginary eigenvalues. The proof is based on the Orlando formula and Hurwitz determinant.

Lemma 3.2: [28] Consider matrix Jac in (6) with characteristic polynomial $p(s)$ in (7). If $p(s)$ satisfies the conditions $\triangle_{n-1} = 0$, then matrix Jac will have a pair of imaginary eigenvalues with multiplicity not greater than one.

We can now express the conditions for jacobian eigenvalues in table I in term of parameter $\mu = (\lambda, k)$. Let Ω^{SN} be the set of parameter for which a saddle node bifurcation occurs. Using the conditions in proposition 3.1, we have that

$$\Omega^{SN} = \{\mu \in \mathbb{R}^m | a_n = 0, a_{n-1} \neq 0\}. \tag{8}$$

Note that Ω^{SN} also describes the parameters where pitchfork and transcritical bifurcations occur. In a similar way, lemma 3.2 can be used to describe the parameter set Ω^H where hopf bifurcation occurs

$$\Omega^H = \{\mu \in \mathbb{R}^m | \triangle_{n-1} = 0\}. \tag{9}$$

Given the sets Ω^{SN} and Ω^H, we can define the parameter set for which at least one type of bifurcation occurs as follows.

$$\Omega = \Omega^{SN} \cup \Omega^H. \tag{10}$$

Thus, system (2) will undergoes bifurcation if Ω is not empty.

IV. Bifurcation-free parameter set & distance to bifurcation

We note from the previous section that the conditions for the existence of a particular bifurcation can be specified by the nonemptiness of the corresponding bifurcation set. In particular, these sets are described as semialgebraic sets in the parameter space. This section presents a computational method that can be used to check the emptiness/nonemptiness of these sets and to compute the minimum distance to bifurcation γ from a given initial values of the parameters. This method is based on *positivstellensatz* from real algebraic geometry [12], [13] and the SOS relaxation method in semidefinite programming [14].

A. The Positivstellensatz

The positivstellensatz (psatz) is a generalization of the *Hilbert's nullstellensatz* [21] for polynomials defined over the real field. It gives a sufficient condition for the infeasibility of *real* solutions to a system of polynomial equality/inequality. The main attracting feature of psatz is that it provides an *certificate* or *refutation* for such infeasibility.

Let $\mathbb{R}(k)[x]$ be polynomial ring and consider finite families of polynomials $\{f_j\}_{j=1,\ldots,s}, \{g_i\}_{i=1,\ldots,t}, \{h_l\}_{l=1,\ldots,u} \in \mathbb{R}(k)[x]$. The *ideal* $I(h)$ generated by h_l is the set

$$I(h) = \{\Sigma_{l=1}^u \mu_l h_l, \text{ for } \mu_l \in \mathbb{R}(k)[x]\}.$$

The *multiplicative monoid* $\mathcal{M}(g)$ generated by $g_i(x)$ is the set of all finite products of $g_i(x)$'s including the identity and the empty products. The *algebraic cone* $\mathcal{C}(f)$ generated by f_j is the set

$$\mathcal{C}(f) = \{p_0 + \Sigma_{j=1}^s p_j F_j \text{ with } p_j \in \mathcal{P}_n^{2d}, F_j \in \mathcal{M}(f)\}.$$

Theorem 4.1 (Positivstellensatz, [12]): Let $\{f_j\}$, $\{g_i\}$, and $\{h_l\}$ be finite families of polynomials in $\mathbb{R}(k)[x]$. Then, the following properties are equivalent

- The set
$$\{x \in \mathbb{R}^n(k) | f_j \geq 0,\ g_i \neq 0,\ h_l = 0\}, \tag{11}$$
is empty.
- There exist $f \in \mathcal{C}(f), g \in \mathcal{M}(g), h \in \mathcal{I}(h)$ such that $f + g^2 + h = 0$.

The psatz essentially gives a sufficient condition for the nonexistence of solutions to a system of polynomial equations/inequation and inequalities. Such nonexistence is certified by the psat refutation in form of polynomials f, g and h. As shown in [14], the search of the psatz refutation can be cast as an SOS program and solved efficiently using SOSTOOLS and Sedumi [15], [16].

B. Characterization of bifurcation-free parameter set

Consider the set Ω^{SN} in (8). Let $\beta_1 > 0$ be a constant and let $V_1(\mu)$ be polynomial in the unknown μ. Consider the set

$$\tilde{\Omega}^{SN} = \{\mu \in \mathbb{R}^m | V_1(\mu) \leq \beta_1\},$$

which satisfies $\tilde{\Omega}^{SN} \cap \Omega^{SN} = \varnothing$. The set $\tilde{\Omega}^{SN}$ can be interpreted as a subset in the parameter space (defined by the level set $V_1(\mu) \leq \beta_1$) at which no saddle node bifurcation will occur. The following proposition characterizes the set $\tilde{\Omega}^{SN}$ by the level set of $V_1(\mu)$.

Proposition 4.2: Consider the set Ω^{SN} in (8). Suppose there exists polynomials $V_1(\mu)$ and $r(\mu)$ and a constant $\beta_1 > 0$ such that

$$a_{n-1}^2(\mu)(V_1(\mu) - \beta_1) + r(\mu)a_n(\mu) \quad \text{is SOS.} \tag{12}$$

Let $\tilde{\Omega}^{SN} = \{\mu \in \mathbb{R}^m | V_1(\mu) \leq \beta_1\}$. Then $\Omega^{SN} \cap \tilde{\Omega}^{SN} = \varnothing$.

Proof: Verifying the condition $\Omega^{SN} \cap \tilde{\Omega}^{SN} = \varnothing$ amounts to check the emptiness of the set

$$\{\mu | a_n = 0, a_{n-1} \neq 0, V_1(\mu) - \beta_1 \neq 0, -(V_1(\mu) - \beta_1) \geq 0\}.$$

Using the psatz theorem, the emptiness of this set is guaranteed by the existence of SOS polynomials s_0, s_1, polynomials $V_1(\mu), t(\mu)$ and constant $\beta_1 > 0$ such that

$$s_0 - s_1(V_1(\mu) - \beta_1) + a_{n-1}^{2m}(V_1(\mu) - \beta_1)^{2m} + t(\mu)a_n = 0.$$

Let $s_0 = 0, m = 1$, and $t(\mu) = (V_1(\mu) - \beta_1)r(\mu)$. We have

$$s_1(V_1(\mu) - \beta_1) = (V_1(\mu) - \beta_1)\left[a_{n-1}^2(V_1(\mu) - \beta_1) + r(\mu)a_n\right],$$

which implies the SOS condition in (12). Now consider any $\mu \in \Omega^{SN}$ for which the condition $a_n(\mu) = 0$ is satisfied. Upon substitution with the SOS condition in (12), we have

$$a_{n-1}^2(\mu)(V_1(\mu) - \beta_1) \geq 0.$$

Since $a_{n-1}^2 > 0$, we have that $V_1(\mu) - \beta_1 \geq 0$ which implies that any $\mu \in \Omega^{SN}$ will lies outside the level set defined by $V_1(\mu) \leq \beta_1$. ■

In a similar way, we can define the parameter set $V_2(\mu)$ at which no hopf bifurcation will occur. For $\beta_2 > 0$ be a constant and define the set

$$\tilde{\Omega}^H = \{\mu \in \mathbb{R}^m | V_2(\mu) \leq \beta_2\},$$

such that $\tilde{\Omega}^H \cap \Omega^H = \varnothing$. The level set $\tilde{\Omega}^H$ can also be characterized in term of the level set of $V_2(\mu)$.

Proposition 4.3: Consider the set Ω^H in (9). Suppose there exists polynomials $V_2(\mu)$ and $r(\mu)$ and constant $\beta_2 > 0$ such that

$$V_2(\mu) - \beta_1 + r(\mu)\triangle_{n-1}(\mu) \quad \text{is SOS.} \tag{13}$$

Let $\tilde{\Omega}^H = \{\mu \in \mathbb{R}^m | V_2(\mu) \leq \beta_2\}$. Then $\Omega^H \cap \tilde{\Omega}^H = \varnothing$.

Proof: Verifying the condition $\Omega^H \cap \tilde{\Omega}^H = \varnothing$ amounts to check the emptiness of the set

$$\{\mu | \triangle_{n-1} = 0, V_2(\mu) - \beta_1 \neq 0, -(V_2(\mu) - \beta_2) \geq 0\}.$$

Using the psatz theorem, this set is empty if there exist SOS polynomials s_0 and s_1, polynomials $V_2(\mu)$ and $t(\mu)$, and a constant $\beta_2 > 0$ such that

$$s_0 - s_1(V_2(\mu) - \beta_1) + (V_2(\mu) - \beta_2)^{2m} + t(\mu)\triangle_{n-1} = 0.$$

Let $s_0 = 0, m = 1, t(\mu) = (V_2(\mu) - \beta_2)r(\mu)$, we then have

$$s_1(V_2(\mu) - \beta_2) = (V_2(\mu) - \beta_2)\left[(V_2(\mu) - \beta_2) + r(\mu)\triangle_{n-1}\right],$$

which implies the SOS condition in (13). Now consider any $\mu \in \Omega^H$ for which the condition $\triangle_{n-1}(\mu) = 0$ is satisfied. Substitution to the SOS condition in (13) gives $V_2(\mu) > \beta_2$ which implies that any $\mu \in \Omega^H$ lies outside the level set defined by $V_2(\mu) \leq \beta_2$. ■

Using the level sets $V_1(\mu)$ and $V_2(\mu)$, the sublevel set in the parameter space at which no bifurcation occur is defined by $\tilde{\Omega} = \min(\beta_1, \beta_2)$. Each of the bound $b_i,\ (i = 1, 2)$ can be computed using SOS program to obtain the level set of the form $V_i(\mu) \leq \beta_i$. For example, the SOS program to compute the set $V_1(\mu) \leq \beta_1$ is given by

$$\begin{array}{ll} \max & \beta_1 \\ \text{s.t.} & a_{n-1}^2(\mu)(V_1(\mu) - \beta_1) + r(\mu)a_n(\mu) \quad \text{is SOS.} \end{array}$$

In this SOS program, both $V_1(\mu)$ and $r(\mu)$ are polynomials parameterization of fixed order and their coeficients will be solved during the optimization. It can be solved eficiently using SOSTOOLS and Sedumi [15], [16].

C. Minimum distance to bifurcation

The SOS program described in the previous section shows that the maximum value of β_i gives the maximum bifurcation-free parameter set $V_i(\mu)$. Now let μ^0 denotes the initial parameter values for system (2) such that $\mu^0 \in V_i(\mu)$, and let μ^* denotes the critical parameter value at which a bifurcation occur. Consider the case that $V_i(\mu)$ takes the form $V_i(\mu) = |\mu^* - \mu^0|$, which also define the distance between μ^0 and μ^*. Then the minimum distance to bifurcation between an initial parameter μ^0 and the critical parameter μ^* can be computed as follows.

Proposition 4.4: Consider system (2) and its Jacobian matrix defined in (6). Let μ^0 be the initial parameters and let μ^* denotes the critical parameters at which a saddle node bifurcation occur. If there exists a constant $\bar{\beta}_1 > 0$, polynomials $\bar{V}_1 = |\mu^* - \mu^0|$ and $r(\mu)$ such that the following SOS program

$$\begin{array}{ll} \max & \bar{\beta}_1 \\ \text{s.t.} & a_{n-1}^2(\mu)(\bar{V}_1(\mu) - \beta_1) + r(\mu)a_n(\mu) \quad \text{is SOS,} \end{array}$$

has a feasible solution, then the distance to bifurcation is defined as $|\mu^* - \mu^0| \geq \beta_1$.

Proof: From proposition 4.2, we know that the maximum value of $\bar{\beta}_1$ defines the maximum distance $|\mu^* - \mu^0|$ at which no saddle node bifurcation exit. Equivalently, this means that $\bar{\beta}_1$ serves as a lower bound for the distance to bifurcation from an initial parameter μ^0. ■

V. Example

The method for identifying the set of bifurcation-free parameter and the computation of minimum distance to bifurcation described in the previous sections will be applied to analyze a tritrophic food chain model described in [29].

A. Model

Consider a tritrophic food chain model described by the following state equation [29].

$$\begin{aligned} \dot{x}_1 &= x_1(1 - x_1) - \frac{k_1 x_1 x_2}{k_2 + x_1}, \\ \dot{x}_2 &= \frac{k_3 x_1 x_2}{k_2 + x_1} - k_4 x_2 x_3 - k_5 x_2, \\ \dot{x}_3 &= k_6 x_2 x_3 - k_7 x_3, \end{aligned} \tag{14}$$

where x_1, x_2, x_3 denote the population density of primary producer, primary consumer, and top predator, respectively. The initial condition is denoted by $x_0 = (x_{10}, x_{20}, x_{30})^T$. The primary producer grows according to the standard logistic growth function and consumed by the primary consumer according to the Holling type II response function with efficient consumption rate k_1. Parameter $k_1(k_6)$ describes the consumption rate of predator (super-predator) on prey (predator), whereas $k_5(k_7)$ denote the death rate of predator (super-predator). We first transform (14) into an equivalent model defined on the ring $\mathbb{R}(k)[x]$. Introducing an extra state variable $x_4 = k_2 + x_1$ to model (14), we have

$$\dot{x}_4 = \frac{\partial(k_2 + x_1)}{\partial x_1}\dot{x}_1 = x_1 x_4^2(x_1 - 1) + k_1 x_1 x_2 x_4^3.$$

The augmented model is now given by

$$\begin{aligned} \dot{x}_1 &= x_1(1 - x_1) - k_1 x_1 x_2 x_4, \\ \dot{x}_2 &= k_3 x_1 x_2 x_4 - k_4 x_2 x_3 - k_5 x_2, \\ \dot{x}_3 &= k_6 x_2 x_3 - k_7 x_3, \\ \dot{x}_4 &= x_1 x_4^2(x_1 - 1) + k_1 x_1 x_2 x_4^3, \end{aligned} \tag{15}$$

with initial condition $x_0 = (x_{10}, x_{20}, x_{30}, (k_2 + x_{10})^{-1})^T$. Thus, matrix N and vector $v(x, k)$ in equation (2) are

$$N = \begin{bmatrix} 1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 \end{bmatrix},$$

$$v(x,k) = [x_1, x_1^2, k_1x_1x_2x_4, k_3x_1x_2x_4, k_4x_2x_3, k_5x_2, k_6x_2x_3, k_7x_3, x_1^2x_4^2, x_1x_4^2, k_1x_1x_2x_4^3]^T.$$

One can veriy that matrix N has a full row rank and therefore no conservation relation exist (i.e. $W = 0$ in (2)). The matrix Z which satisfy $v(x,k) = diag(k)x^Z$ is

$$Z = \begin{bmatrix} 1 & 2 & 1 & 1 & 0 & 0 & 0 & 0 & 2 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 2 & 2 & 3 \end{bmatrix}.$$

For $i = 1, \ldots, 4$, let $h_i = 1/x_i^*$ where x_i^* is the state equilibrium parameterization given by

$$\begin{aligned} x_1^* &= \lambda_6/(\lambda_6+\lambda_7), \quad x_2^* = \lambda_6/k_6(\lambda_6+\lambda_7), \\ x_3^* &= k_6\lambda_7/k_1\lambda_6, \quad x_4^* = k_5\lambda_5(\lambda_6+\lambda_7)^2/\lambda_6^2, \end{aligned} \quad (16)$$

which are obtained using the technique described in appendix B. The jacobian matrix (6) for system (15) is given by

$$\begin{aligned} Jac &= N\text{diag}(E\lambda)Z^T\text{diag}(h) \\ &= \begin{bmatrix} -h_1\lambda_1 & -h_2\lambda_2 & 0 & -h_4\lambda_2 \\ h_1(\lambda_3+\lambda_4) & 0 & -h_3\lambda_3 & h_4(\lambda_3+\lambda_4) \\ 0 & h_2\lambda_5 & 0 & 0 \\ h_1\lambda_6 & h_2\lambda_7 & 0 & h_4\lambda_7 \end{bmatrix} \end{aligned}$$

with characteristic polynomial

$$s^4 + a_1s^3 + a_2s^2 + a_3s + a_4 = 0,$$

where $a_1 = h_1\lambda_1 - h_4\lambda_7$ and

$$\begin{aligned} a_2 = {} & h_2h_3\lambda_3\lambda_5 + h_2(\lambda_3+\lambda_4)(h_1\lambda_2 - h_4\lambda_7) \\ & + h_1h_4(\lambda_2\lambda_6 - \lambda_1\lambda_7), \\ a_3 = {} & h_2h_3\lambda_3\lambda_5(h_1\lambda_1 - h_4\lambda_7) + h_1h_2h_4(\lambda_2\lambda_3\lambda_6 \\ & + \lambda_2\lambda_4\lambda_6 - \lambda_1\lambda_3\lambda_6 - \lambda_1\lambda_4\lambda_7) \\ a_4 = {} & h_1h_2h_3h_4(\lambda_2\lambda_6 - \lambda_1\lambda_7). \end{aligned}$$

The first three Hurwitz determinants are $\triangle_1 = a_1$, $\triangle_2 = a_1a_2 - a_3$, $\triangle_3 = a_1(a_2a_3 - a_1a_4) - a_3^2$.

B. Minimum distance to bifurcation

Let $x_0 = (x_1^0, x_2^0, x_3^0) = (0.7, 0.8, 1.4)$ be an initial condition and let $k^0 = (0.4, 0.4, 0.25, 0.1, 0.02, 0.25, 0.2)$ be an initial parameter. One can verify that this initial condition is an asymptotically stable equilibrium point. Using the equilibrium parameterization in (16), the initial convex parameters are $\lambda^0 = (0.1, 0.25, 0.084, 0.016, 0.21, 0.25, 0.1)$. The combined parameter that will be used to compute γ are $\mu^0 = (k_1, k_5, k_6, \lambda_3, \lambda_5, \lambda_6, \lambda_7)$. We aim to compute the minimum distance γ from k^0 to the nearest hopf bifurcation point. Using Jacobian matrix Jac, the necessary condition for hopf bifurcation in lemma 3.2 is $\triangle_{n-1}(\mu) = 0$ with

$$\triangle_{n-1}(\mu) = h_1h_2h_3h_4\lambda_3\lambda_5(\lambda_2\lambda_6 - \lambda_1\lambda_7).$$

Since $h_i \geq 0$, $(i = 1, \ldots, 4)$ and $\lambda_j \geq 0$, $(j = 1, \ldots, 7)$, this condition can be simplified as $\lambda_2\lambda_6 - \lambda_1\lambda_7 = 0$. Thus, the SOS program takes the form

$$\begin{aligned} &\max \quad \bar{\beta}_2 \\ &\text{s.t.} \quad V_2(\mu) - \bar{\beta}_2 + r(\mu)\triangle_{n-1}(\mu) \quad \text{is SOS.} \end{aligned}$$

where $V_2(\mu) = \sum(\mu_i^0 - \mu_i^*)^2$, for $i = 1, \ldots, 7$. Using SOSTOOLS and Sedumi, we get a minimum distance of $\gamma = 0.142$ which corresponds to critical parameters $k^* = (0.02, 0.4, 0.25, 0.1, 0.0002, 0.2766, 0.18)$.

APPENDIX

A. Basic Algebraic Geometry

These materials can be found in standard algebraic geometry literature such as [21]. Consider polynomial ring $\mathbb{C}(k)[x]$. The set $I \subseteq \mathbb{C}(k)[x]$ is an *ideal* if it satisfies: (i) $0 \in I$, (ii) $\forall a, b \in I \Rightarrow a + b \in I$, and (iii) $\forall a \in I, b \in \mathbb{C}(k)[x] \Rightarrow a \cdot b \in I$. Let $f_1, \ldots, f_q$ be polynomials in $\mathbb{C}(k)[x]$. We set

$$\begin{aligned} I &= \{\Sigma_{i=1}^q h_if_i, \text{ with } h_i \in \mathbb{C}(k)[x]\}, \\ &= \langle f_1, \ldots, f_q\rangle \subset \mathbb{C}(k)[x]. \end{aligned}$$

One can show that I is an *ideal* called the *ideal generated by* $f_1, \ldots, f_q$. Correspondingly, the polynomials $f_1, \ldots, f_q$ are called the *basis* of I. The zeros of an ideal I is called its *affine variety*, i.e. for $I = \langle f_1, \ldots, f_q\rangle$, the set

$$\begin{aligned} V(I) &= \{x \in \mathbb{C}^n(k) : \ f_i(x) = 0, \text{ for all } 1 \leq i \leq q\}, \\ &= V(f_1, \ldots, f_q), \end{aligned}$$

is the *affine variety* of I defined by $f_1, \ldots, f_q$. An affine variety is the set of solution to system of polynomial equation.

Given ideal I, the existence of its complex solution can be proved using Hilbert's Nullstellensatz.

Theorem 1.1 (Hilbert's Nullstellensatz): Let $(f_j)_{j=1,\ldots,s}$ be finite family of polynomials in $\mathbb{C}(k)[x]$. Let I be the ideal generated by (f_j). The following statements are equivalent:

- The set $\{x \in \mathbb{C}^n(k) | f_j = 0, \ j = 1, \ldots, s\}$ is empty.
- The polynomial 1 belongs to ideal I, i.e., $1 \in I$.
- $I = \mathbb{C}(k)[x]$.
- There exist polynomials $g_i \in \mathbb{C}(k)[x]$ such that $f_1(x,k)g_1(x,k) + \cdots + f_s(x,k)g_s(x,k) = 1$.

The nullstellensatz basically states that if there exist polynomials g's satisfying the last statement, then the set of complex solutions $\{x \in \mathbb{C}^n(k) | f(x,k) = 0\}$ is empty. In particular, such emptiness is certified by the existence of polynomials g's. The generalization of nullstellensatz for polynomial ring over the real field is the *positivstellensatz* (section IV-A).

If such solutions are known to exist, they can be computed using the method of Gröbner basis. This method is based on the fundamental result in algebraic geometry which states that the zeros of the basis elements of an ideal I is equivalent to the zeros of the whole ideal I. Since the Hilbert's Basis Theorem guarantees the existence of finite basis for every ideal I, the zeros of an ideal can be computed usiing the zeros o its basis elements. Gröbner basis with elimination ordering is an important basis for such purpose since its zeros can often be solved easily using standard back substitution procedure. Gröbner basis can be computed using the standard Buchberger algorithm which has been implemented in many computer algebra software [22]. Computing the zeros of an ideal I using Gröbner basis method consists of two main steps namely the *elimination* and the *extension* steps.

1) Elimination: This step aims to compute the rth elimination ideal I_r of I whose zeros can be solved easily.

Definition 1.2: Given $I = \langle f_1, \ldots, f_q \rangle \subset \mathbb{C}(k)[x]$, the rth elimination ideal $I_r \subset \mathbb{C}(k)[x_{r+1}, \ldots, x_n]$ defined by

$$I_r = I \cap \mathbb{C}(k)[x_{r+1}, \ldots, x_n].$$

The Elimination Theorem provides a method to compute a Gröbner basis for the rth elimination ideal I_r.

Theorem 1.3 (Elimination): Let $I \subset \mathbb{C}(k)[x]$ and let G be a Gröbner basis of I with respect to the lex order $x_1 >_{lex} x_2 >_{lex} \cdots >_{lex} x_n$. Then, for every $0 \leq r \leq n$, the set

$$G_r = G \cap \mathbb{C}(k)[x_{r+1}, \ldots, x_n]$$

is a Gröbner basis of the rth elimination ideal I_r.

The variety $V(I_r)$ of elimination ideal I_r can be obtained from its Gröebner basis G_r. $V(I_r)$, however, is a subvariety of the original ideal I (i.e. $V(I_r) \subset V(I)$) and therefore serves only as partial solution to I.

2) Extension: The extension step aims to extend the partial solution $V(I_r)$ obtained in the elimination step to get the whole solution $V(I)$ for ideal I. The condition that allow this extension is given by the Elimination theorem.

Theorem 1.4 (Extension): Let $I = \langle f_1, \ldots, f_q \rangle \subset \mathbb{C}(k)[x]$ and let I_1 be the first elimination ideal of I. For each $1 \leq i \leq q$, write f_i in the form

$$f_i = g_i(x_2, \ldots, x_q) x_1^{N_i} + \text{ terms where } x_1 \text{ has degree} < N_i, \tag{17}$$

where $N_i > 0$ and $g_i \in \mathbb{C}(k)[x_2, \ldots, x_n]$ is nonzero. Suppose that we have a partial solution $(x_2^*, \ldots, x_n^*) \in V(I_1)$. If $(x_2^*, \ldots, x_n^*) \notin V(g_1, \ldots, g_q)$, then there exists $x_1^* \in \mathbb{C}(k)$ such that $(x_1^*, \ldots, x_n^*) \in V(I)$.

It can be seen that the goal of the elimination step is to iteratively reduces the original problem into problems with smaller number of variables for which the solutions can be computed easily. The extension step then back substitutes these solution to the original problem to get the total solution. The importance of Gröbner basis in this case is that it allows for a systematic execution of the elimination step. Gröbner basis can be computed using Buchberger algorithm which have been implemented in many computer algebra softwares such as Singular [22]. Buchberger algorithm, however, have doubly exponential worst case complexity in the number of unknown variables. As shown in [23], when there are n unknown variables $(x_1, \ldots, x_n)$ and the polynomials in $f(x, k)$ have a total degree not exceeding d, then the degree of polynomials in Gröbner basis G is bounded by $2(\frac{1}{2}d^2 + d)^{2^{n-1}}$. This bound is doubly exponential with respect to n which makes the Buchberger algorithm may require a large memory. Nevertheless, many applications have shown that such worst case bound is not always encountered.

B. Equilibrium parameterization

This section reviews the method proposed in [11], [24] for parameterizing the state equilibrium x^* of (2). It involves computating the parameterized rate equilibrium v^* formed by the intersection of toric variety and convex cone.

1) Toric variety: The approach to compute v^* is based on recognizing that the kernel of the mapping between x and $v(x, k)$ induces an algebraic object known as toric ideal whose variety is called toric variety. Following the two main steps in using Gröbner basis to compute the variety of an ideal, we describe both the elimination and extension steps for parameterizing x^*. The elimination step aims to compute the toric variety which gives the rate equilibrium v^*. This toric variety is then used in the extension step to compute the state equilibrium x^*.

a) The Elimination Step: Let $R(k)[x]$ be a ring in the unknown $x = (x_1, \ldots, x_n)$ and let $R(k)[v]$ be a ring in another unknown $v = (v_1, \ldots, v_m)$. Recall that the mapping $v(x, k)$ between $x \in \mathbb{R}^n$ and $v \in \mathbb{R}^m$ in (2) is given by

$$v(x, k) : \mathbb{R}_+^n \mapsto \mathbb{R}_+^m, \quad x \mapsto v = kx^Z$$

with the image of $v(x, k)$ is defined as

$$v_1(x, k) = k_1 x^{Z_1}, \ldots, v_m(x, k) = k_m x^{Z_m}.$$

A given $v^* \in \mathbb{R}_+^m$ will correspond to an $x^* \in \mathbb{R}_+^n$ if the condition $v^* \in \text{im}(v(x^*, k))$ is satisfied (i.e. if v^* lies on the image of the map $v(x^*, k)$). This condition can be checked by evaluating the zeros of the expressions

$$v_i - v_i(x, k), \quad \text{for } i = 1, \ldots, m. \tag{18}$$

The expression in (18) is binomial ideal on $\mathbb{R}(k)[x, v]$. The rate equilibrium v^*, however, lies on the variety of a toric ideal $\mathcal{I} = \langle v_i - v_i(x, k) \rangle \cap \mathbb{R}(k)[v]$ (note the difference of the ring) and is called toric variety $V(\mathcal{I})$. Using Elimitation Theorem, a Gröbner basis for $\mathcal{I}$ can be computed from the Gröbner basis of binomial ideal (18) in the following way.

First, define ideal $I \in \mathbb{R}(k)[x, v]$ corresponding to (18)

$$I = \langle v_1 - k_1 x^{Z_1}, \ldots, v_m - k_m x^{Z_m} \rangle \in \mathbb{R}(k)[x, v]. \tag{19}$$

The corresponding toric ideal $\mathcal{I} \in \mathbb{R}(k)[v]$ is given by

$$\begin{aligned} \mathcal{I} &= \langle v_1 - k_1 x^{Z_1}, \ldots, v_m - k_m x^{Z_m} \rangle \cap \mathbb{R}(k)[v], \\ &= I \cap \mathbb{R}(k)[v]. \end{aligned} \tag{20}$$

By Hilbert's Basis Theorem, I is generated by a finite number of basis and one choice of such basis is the Gröbner basis. Since $I \in \mathbb{R}(k)(x, v)$ is a binomial ideal, its Gröbner basis will also be binomial defined on $\mathbb{R}(k)(x, v)$ [30], [22]. Let G denotes the Gröbner basis of I with respect to elimination ordering for x. Now notice that the toric ideal $\mathcal{I}$ in (20), obtained from the intersection $I \cap \mathbb{R}(k)[v]$, is the nth elimination ideal of I (as it is computed by eliminating n variables x from I) on $\mathbb{R}(k)[v]$. Using the Gröbner basis G of ideal I, the Elimination Theorem implies that the basis $G_n(v) = G \cap \mathbb{R}(k)[v]$ is a Gröbner basis for $I \cap \mathbb{R}(k)[v] = \mathcal{I}$. This means one of the Gröbner bases for toric ideal $\mathcal{I}$ is those basis in G which only contain variable v. Since the variety of an ideal is equivalent to the variety of its basis, then the toric variety $V(\mathcal{I})$ is given by

$$V(\mathcal{I}) = \{v \in \mathbb{Q}^m(k) : G_n(v) = 0\} \subset \mathbb{R}(k)[v]. \tag{21}$$

The toric variety thus define the rate equilibrium v^*, i.e.

$$v^*(k) \in V(\mathcal{I}). \tag{22}$$

b) The Extension step: By the Ideal-Variety Correspondence theorem [21], we know that any variety $V(I) \in \mathbb{R}(k)[x,v]$ of binomial ideal (19) must vanish on $v^*(k) \in \mathbb{R}(k)[v]$ in (22). Thus, $v^*(k)$ in (22) is a partial solution to $V(I)$ and we need to extend it to get the remaining solution x^* which then define the total solution $V(I) \subset \mathbb{R}(k)[x,v]$.

The existence of this extension can be shown using the Extension Theorem. First, rewrite the ideal in (19) as

$$v^* = \text{diag}(k)(x^*)^Z.$$

For given nonzero partial solution $v^*(k)$, this representation satisfies equation (17) with $g_i(\cdot) = \text{diag}(k)$ and the second term on the right hand side of (17) equals to zero. By the Extension Theorem, solution to x^* is guaranteed to exist.

In particular, x^* can be computed using Hermite transformation as follows. Introduce a coordinate transformation $x^* = \omega^U$ with $\omega \in \mathbb{R}^n$ and U is a unimodular matrix. Since $v^*(k) = \text{diag}(k)(x^*)^Z$, we have

$$\text{diag}(k)(x^*)^Z = \text{diag}(k)\omega^{UZ} = \text{diag}(k)\omega^H = v^*(k), \quad (23)$$

where we have used the fact that $UZ = H$, with H is the Hermite normal form of matrix Z. For given $v^*(k)$, solving the equation $\text{diag}(k)\omega^H = v^*(k)$ for ω and then followed by computing x^* using relation $x^* = \omega^U$, the solution $x^*(k) \in \mathbb{R}(k)[x]$ can be obtained. Both $x^*(k)$ and $v^*(k)$ then define the variety of binomial ideal I in (19).

2) Convex polyhedral cone: One may see from (2) that the rate equilibrium v^* is confined to a set $\mathcal{K}_v$ defined by

$$v^* \in \mathcal{K}_v = \{\ker(N) \cap \mathbb{R}^m_+\}.$$

$\mathcal{K}_v$ is actually a convex polyhedral cone, generated by linear combinations of finite number (M) of extreme rays, E_i for $i = 1, \ldots, M$ [17], [11]. There are tools that can be used to compute these extreme rays [31]. Since $\mathcal{K}_v$ is convex, there exists $\lambda_i > 0$ such that the cone $\mathcal{K}_v$ can be parameterized as $\mathcal{K}_v = \sum_{i=1}^M \lambda_i E_i$, where λ is convex parameters. Thus, the rate equilibrium v^* can also be parameterized by convex parameter λ_i [17], [11]

$$v^*(\lambda) = \sum_{i=1}^{M} \lambda_i E_i. \quad (24)$$

Given the parameterization (22) and (24), the rate equilibrium of system (2)is then defined as their intersection, i.e.

$$v^*(\lambda, k) = \{v^* \in V(\mathcal{I})\} \cap \{v^* \in \mathcal{K}_v\} \subset \mathbb{R}(\lambda, k)[v]. \quad (25)$$

By substituting this intersection to (23), the parameterized state equilibrium $x^*(\lambda, k)$ can also be obtained. The complete algorith to compute $v^(\lambda, k)$ in (25) is depicted on figure 1. Gröbner basis for binomial ideal of the form (18) (step 4 in figure 1) can be computed using Singular [22].

1: **Input**: rate vector, $v(x,k) = (k_1 x^{Z_1}, \ldots, k_m x^{Z_m})^T$
2: **Output**: parameterized state equilibrium, $x^*(\lambda, k)$
3: Construct ideal $I \subset \mathbb{R}(k)[x,v]$ in (19) as
$$I = \langle v_1 - k_1 x^{Z_1}, \ldots, v_m - k_m x^{Z_m} \rangle \in \mathbb{R}(k)[x,v].$$
4: Compute a Gröbner basis G of I using lex order $x_1 > \cdots > x_n > v_1 \cdots > v_m$. (Tools: [22])
5: Compute the Gröbner basis $G_n \in \mathbb{R}(k)[v]$ for the nth elimination ideal of I according to
$$G_n = G \cap \mathbb{R}(k)[v],$$
i.e. G_n contains those basis in G that depend only on v. The toric ideal in (20) becomes $\mathcal{I}\langle G_n \rangle \subset \mathbb{R}(k)[v]$. Its variety is $V(\mathcal{I}) = \{v \in \mathbb{R}(k)^m : G_n = 0\} \subset \mathbb{R}(k)[v]$.
6: The rate equilibrium is then defined as $v^*(k) \in V(\mathcal{I})$.
7: Compute the convex parameterization of rate equilibrium $v^*(\lambda) \in \mathcal{K}_v$. (Tools: [31])
8: The rate equilibrium is formed by the intersection
$$v^*(\lambda, k) = \{v^* \in V(\mathcal{I})\} \cap \{v^* \in \mathcal{K}_v\}.$$
9: Use Hermite transformation (23) to compute $x^*(\lambda, k)$.

Fig. 1: Parameterization of state equilibrium $x^*(\lambda, k)$.

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