The Distance-to-Bifurcation Problem in Non-negative Dynamical Systems with Kinetic Realizations

Tua A. Tamba and M.D. Lemmon

Abstract—Consider a dynamical system \( \dot{x} = f(x,k_0) \) whose vector field is parameterized by real parameters \( k_0 \). The distance-to-bifurcation problem seeks the smallest parameter variation \( \gamma = |k - k_0| \) that results in a bifurcation of the original system’s phase portrait. Prior work on this problem used numerical methods to search for the minimum \( \gamma \), but these methods were computationally demanding and only guaranteed locally optimal solutions. This paper recasts the minimum distance-to-bifurcation problem as a sum-of-squares (SOS) relaxation for non-negative dynamical systems that have kinetic realizations. The class of systems with kinetic realizations is large enough to characterize a wide range of real world applications and the use of such realizations allows one to find explicit parameterizations of the system Jacobian as a rational function of system parameters. This parameterization of the Jacobian was originally proposed for chemical reaction networks and its value is that it greatly simplifies the distance-to-bifurcation problem by removing the need to keep the system’s equilibria as decision variables in the distance-to-bifurcation problem. The proposed approach is illustrated on an food web in aquatic eco-systems. The example demonstrates that our approach is able to identify how a coordinated set of parameter variations may result in a smaller distance-to-bifurcation than predicted by competing computational tools.

I. INTRODUCTION

Many real life systems are subject to external perturbations that cause systems parameters to vary away from the nominal values. For nonlinear systems, such parameter variations 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 non-equivalent phase portrait of the system [1]. In many cases, these changes come with catastrophic effects. For example, load variations in power networks may induce a saddle node bifurcation that causes a voltage collapse [2], [3]. Another example occurs in shallow lakes where increased nutrient loading may result in a pitchfork bifurcation that shifts a previously clear lake with high biodiversity into a turbid lake dominated by algae [4]. Each of these effects has the potential to disrupt the services that these systems provide to society. Understanding the resilience of these systems to parameter variations 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 parameter \( k^* \) at which a bifurcation occur. The quantity \( \gamma \), often called distance to closest bifurcation, is an indicator of how close the system is to a collapse. The computation of \( \gamma \) is generally difficult since the bifurcation set containing \( k^* \) is usually unknown. For dynamical systems

\[ \dot{x} = f(x,k), \]  

whose equilibrium \( x^* \) depend on parameter \( k \), the bifurcation set consists of those parameters that satisfy the bifurcation conditions in Table I. The first row of the table shows necessary and sufficient conditions for a Hopf bifurcation. The transversality condition requires that the partial derivative (with respect to parameter \( k \)) of the real part of the characteristic polynomials root be not equal to zero. The other transversality conditions in this table are conditions on the various derivatives of the vector field in which \( v \) and \( w \) are the left and right eigenvectors, respectively, associated with the zero eigenvalue of the Jacobian matrix. Previous works have proposed several methods for computing \( \gamma \) 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 \( \gamma \) 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 \( \gamma \) requires the computation of equilibrium \( x^* \) at every iteration.

<table>
<thead>
<tr>
<th>Type</th>
<th>Jacobian Eigenvalue</th>
<th>Transversality</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hopf</td>
<td>simple 0</td>
<td>( D_k { \text{Re}(\alpha) } \neq 0 )</td>
</tr>
<tr>
<td>Saddle node</td>
<td>simple imaginary pair</td>
<td>( w^T \left( D_k f \big</td>
</tr>
<tr>
<td>Transcritical</td>
<td>simple imaginary pair</td>
<td>( w^T \left( D_k f \big</td>
</tr>
<tr>
<td>Pitchfork</td>
<td>simple imaginary pair</td>
<td>( w^T \left( D_k f \big</td>
</tr>
</tbody>
</table>

This paper uses sum-of-squares (SOS) relaxations [11], [12] to bound the "distance-to-bifurcation", \( \gamma \), in a class of non-negative dynamical systems that have kinetic realizations. A dynamical system \( \dot{x} = f(x,k) \) has a kinetic realization if there exists a matrix \( N \) and a vector of monomials \( v(x,k) \) with variables \( x \) and parameters \( k \) such
that \( f(x, k) = Nv(x, k) \). These realizations often occur in chemical reaction networks and their special structure allows one to compute an analytical parameterization of the equilibrium in terms of the system parameters. This equilibrium parameterization was first introduced in the context of stoichiometric network analysis and is based on the concept of a toric variety [13], [14]. This parameterization of the equilibria simplifies the distance-to-bifurcation problem in that the constraints are then expressed only in terms of the parameters, rather than the parameters and the equilibria. This paper uses an SOS relaxation [11], [12] to obtain a lower bound on the globally minimum distance to bifurcation and illustrates the application of this method to study bifurcations in an aquatic food web.

The remainder of the paper is structured as follows. Section II describes kinetic realizations of dynamical systems. Section III describes necessary conditions for bifurcations that are then used in section IV to recast the distance-to-bifurcation problem as a sum-of-squares (SOS) relaxation. 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 \( i \)th component of that vector. An \( n \)-dimensional multi-index is an \( n \)-tuple, \( \alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n) \) of non-negative integers. The absolute value of a multi-index \( \alpha \) 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 \( \alpha \), 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 \( p \)th order polynomial in \( n \) unknowns \( x = (x_1, \ldots, x_n) \) with coefficients \( k = (k_1, \ldots, k_p) \) in the field \( \mathbb{F} \) is a finite linear combination of monomials of the form

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

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 \( f(x, k) \geq 0, \forall x \in \mathbb{R}^n \). 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 \( q_i(x, k) \in \mathbb{R}(x, k) \). Clearly, an SOS polynomial is also psd.

**II. KINETIC REALIZATIONS**

Consider an \( n \)-dimensional polynomial system whose state trajectories \( x(t, x_0) \) satisfy

\[
 \dot{x}(t) = f(x(t), k), \quad x(0) = x_0, \quad (2)
\]

for all \( t \geq 0 \) in which \( f(x, k) \in \mathbb{R}^n(k)[x] \). This system is non-negative if and only if for all \( x_0 \in \mathbb{R}^n_0 \) then \( x(t, x_0) \in \mathbb{R}^n_+ \) for all \( t \geq 0 \). A necessary and sufficient condition for (2) to be non-negative is that \( f(x, k) \geq 0 \) for all \( x \) in which \( x_i = 0 \) [15].

The system in (2) has a kinetic realization if there exists an \( n \times m \) real matrix, \( N \), and an \( m \times 1 \) vector of monomials, \( v(x, k) \), in \( \mathbb{R}(k)[x] \) such that

\[
 \dot{x}(t) = f(x, k) = Nv(x, k), \quad x(0) = x_0. \quad (3)
\]

In general the matrix \( N \) is sparse and the vector \( v(x, k) \) is a vector of fluxes within the system. The flux vector can be decomposed as \( v(x, k) = \text{diag}(k)x^2 \), with \( Z \in \mathbb{Z}_+^{n \times m} \) being a matrix with its \( i \)th column is the multi-index of the \( i \)th monomial in \( v(x, k) \).

Non-negative systems exist for a large number of real world systems including compartmental systems, biological systems, ecological systems [16]. The restriction to polynomial systems with kinetic realizations is not overly restrictive since 1) any smooth function can be approximated arbitrarily closely with a polynomial [17], 2) systems with rational vector fields can be transformed into polynomial systems [18], and 3) there exist a number of approaches for extracting kinetic realizations from polynomial systems [19], [20], [21], [22], [23], [24].

The system’s equilibria are vectors in \( \mathbb{Q}^n(k) \) that are zeros of the right hand side of (3). In other words, \( x^*(k) \) is an equilibrium if

\[
 x^*(k) \in \{ x \in \mathbb{Q}^n(k) : Nv(x, k) = 0 \}. \quad (4)
\]

Computing the algebraic expression for \( x^*(k) \) in high dimensional systems usually requires the use of symbolic methods. These methods are based on the fact that a set of polynomials generate an ideal in the polynomial ring and that the zeros of the system of polynomials are equivalent to the zeros of any Gröbner basis of that ideal. The value of the Gröbner basis is that one can formulate computational methods for systematically solving for the system’s zeros in a manner that is very reminiscent of back-substitution methods used in solving systems of linear algebraic equations. The main stumbling block is that the complexity of computing a Gröbner basis using the Buchberger algorithm [25] is known to grow in a doubly exponential manner with respect to the number of unknown variables [26].

This complexity can be reduced by taking advantage of the special structure of the vector fields in (3) [13], [14] and in doing this one obtains a less complex formulation of the distance-to-bifurcation problem. The special structure in (3) means that the system’s vector fields \( f(x, k) \) may be decomposed into a linear map \( (N) \) which is independent of \( x \) and \( k \) and a vector of nonlinear fluxes \( (v) \). This decomposition has two important consequences that were originally exploited in [13], [14].

**First:** it means that the equilibrium fluxes (i.e. those \( v^* \) such that \( Nv^* = 0 \)) are non-negative vectors lying in the null
space of \( N \). In particular, any equilibrium flux must lie in a convex polyhedral cone

\[
v^* \in K_v = \ker(N) \cap \mathbb{R}_+^m = \left\{ v \in \mathbb{R}_+^m : v = \sum_{i=1}^q \lambda_i E_i \right\}.
\]

The cone, \( K_v \), in equation (5) is finitely generated by a set of extreme rays, \( E_i \in \mathbb{R}_+^m \) for \( i = 1, 2, \ldots, q \). Such rays are routinely computed using tools such as CellNetAnalyzer [27]. Every equilibrium flux in \( K_v \) can therefore be parameterized with respect to these rays. In equation (5), the parameters \( \lambda = (\lambda_1, \lambda_2, \ldots, \lambda_q) \) are called convex parameters [28] and so any equilibrium flux can be written as \( v^*(\lambda) \) a linear function of the convex parameters.

**Second:** any flux, \( v \), in the system must satisfy the equation

\[
v_i = k_i x^{z_i}, \quad i = 1, 2, \ldots, m,
\]

where \( z_i \) is the \( i \)th column of \( Z \) in (3). The equations in (6) are binomials in \( \mathbb{R}(k)[x, v] \) and this system’s zeros characterize both the equilibrium fluxes, \( v^* \), and the state equilibria \( x^* \). The ideal generated by these binomials is a toric ideal [29] and for such ideals one has efficient algorithms for computing a Gröbner basis [30] which have already been implemented in computer algebra programs such as SINGULAR [31]. One is therefore able to efficiently solve for the equilibria of the system in terms of its equilibrium fluxes and system parameters.

The preceding two consequences of our kinetic realization can be summarized as 1) any equilibrium flux can be expressed as a function, \( v^*(\lambda) \), in terms of the convex parameters and 2) any state equilibrium can be expressed as a rational function, \( x^*(v^*, k) \) of the equilibrium fluxes and the system parameters, \( k \). Using the convex parameterization of \( v^* \), one can therefore parameterize the state system as \( x^*(k, \lambda) \in \mathbb{Q}^n(k, \lambda) \). This algebraic equation characterizes all system equilibria as a function of the system and convex parameters and it provides a critical starting point for characterizing the bifurcation constraints in the distance-to-bifurcation problem.

Another important implication of using kinetic realizations is that the system’s Jacobian matrix \( J \) can now be parameterized as [13], [14]

\[
J(\lambda, k) = N \text{diag}(v^*(\lambda)) Z^T \text{diag}(1/x^*(\lambda, k)).
\]

This implies that the bifurcation condition in table I can be evaluated directly in term of the parameters \( (\lambda, k) \) without having to directly compute the equilibrium \( x^* \) for different \( k \). Earlier work on the distance-to-bifurcation problem always required that one solve for the equilibrium as part of the optimization; this increases the number of decision variables in the problem. By using the parameterization of the Jacobian in (7), the number of decision variables in the distance-to-bifurcation problem is reduced to only consist of a small set of convex parameters, \( \lambda \), and system parameters, \( k \).

### III. Necessary Bifurcation Conditions

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 a bifurcation occurs is usually numerically searched for using continuation methods [1]. This method, however, is limited to low dimensional parameter space \( (p \leq 3) \) because evaluating the bifurcation conditions in Table I require knowledge of system’s equilibrium \( x^* \). The Jacobian matrix \( J \) in (7), however, is parameterized in terms of the system equilibria and so the eigenvalue conditions in Table I can be evaluated without having to explicitly compute the equilibrium \( x^* \). We therefore can obtain a semi algebraic description of the bifurcations conditions in Table I which will be used in the next section to formally state the distance-to-bifurcation problem.

Consider the Jacobian matrix (7). Let \( p(s) = |sI - J| \) be the characteristic polynomial of \( J \) defined as

\[
p(s) = a_0 s^n + a_1 s^{n-1} + \cdots + a_{n-1} s + a_n,
\]

where the coefficients \( a_i(\lambda, k) \) are function of the parameters \( (\lambda, k) \). For notational convenience denote the parameters as \( \mu = (\lambda, k) \). The eigenvalues of \( J \) are given by the roots of \( p(s) \), and one says the matrix \( J \) 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 \( z \)th Hurwitz determinant, \( \Delta_z \), associated with the characteristic polynomial \( p(s) \) is

\[
\Delta_z = \left| \begin{array}{cccc}
| & | & | & | \\
| a_1 & a_2 & \cdots & a_{z-1} \\
| a_0 & a_2 & \cdots & a_{z-2} \\
| \vdots & \vdots & \ddots & \vdots \\
| 0 & 0 & \cdots & a_z \\
\end{array} \right|.
\]

such that

\[
\Delta_1 = |a_1|, \quad \Delta_2 = \left| \begin{array}{cc}
| & | \\
a_1 & a_2 \\
\end{array} \right|, \quad \Delta_3 = \left| \begin{array}{ccc}
| & & | \\
a_1 & a_2 & a_3 \\
0 & a_2 & a_3 \\
\end{array} \right|, \quad \cdots
\]

**Proposition 3.1:** Consider matrix \( J \) in (7) with characteristic polynomial \( p(s) \) in (8). If \( p(s) \) satisfies the conditions \( a_n = 0 \) and \( a_{n-1} \neq 0 \), then matrix \( J \) 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

\[
\frac{\partial p(s)}{\partial s} \bigg|_{s=0} \neq 0,
\]

which will be satisfied when \( a_{n-1} \neq 0 \).

The following lemma from [32] gives the condition for \( J \) to have a simple pair of imaginary eigenvalues. The proof is based on the Orlando formula [33].
Lemma 3.2: [32] Consider matrix $J$ in (7) with characteristic polynomial $p(s)$ in (8). If $p(s)$ satisfies the conditions $\Delta_{n-1} = 0$, then matrix $J$ will have a pair of imaginary eigenvalues with multiplicity not greater than one.

Let us rewrite the conditions in table I in term of parameter $\mu = (\lambda, k)$ of the characteristic polynomial’s (8) coefficients. Let $\rho$ denotes the number of parameters in $\mu$. Let $\Omega^{SN}$ be the set of parameters for which a saddle node bifurcation occurs. Using the conditions in proposition 3.1, one has

$$\Omega^{SN} = \{\mu \in \mathbb{R}_+^\rho | a_n(\mu) = 0, a_{n-1}(\mu) \neq 0\}. \quad (9)$$

Note that $\Omega^{SN}$ 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 $\Omega^{H}$ where Hopf bifurcation occurs

$$\Omega^{H} = \{\mu \in \mathbb{R}_+^\rho | \Delta_{n-1}(\mu) = 0\}. \quad (10)$$

If a bifurcation occurs, then one may denote the parameter set for which at least one type of bifurcation occurs as

$$\Omega = \Omega^{SN} \cup \Omega^{H}. \quad (11)$$

Thus, the system (3) will not have a bifurcation if $\Omega$ is empty. The set in (11) is an algebraic set characterizing those parameters for which a bifurcation can possibly occur. A method for checking whether or not this set is empty is discussed in the next section.

IV. Distance-to-Bifurcation Problem

From the previous section, it should be clear that the non-existence of a particular bifurcation is equivalent to the emptiness of the corresponding bifurcation set. In general, checking the emptiness of $\Omega^{SN}$ can be difficult. In recent years, however, it has proven fruitful to consider convex relaxations of the problem in which one checks for the emptiness of the set $\Omega(\beta) \cap \Omega^{SN}$, where $\Omega(\beta)$ is a semi-algebraic set defined by a positive semi-definite certificate function $V(\mu)$. In particular, let $\beta$ be a real constant and let $\alpha(|\mu - \mu_0|)$ be a class $K$ function in which $\mu$ is the parameter set and $\mu_0$ is a known initial parameter. The certificate set is defined as

$$\hat{\Omega}(\beta) = \{\mu \in \mathbb{R}^\rho : \alpha(|\mu - \mu_0|) \leq \beta\}. \quad (12)$$

Given a specific $\beta > 0$, if the intersection of the certificate set $\hat{\Omega}(\beta)$ with the bifurcation set $\Omega^{SN}$ is empty, then the distance to bifurcation cannot be less than $\alpha^{-\frac{1}{\beta}}(\beta)$. The key point is that verifying whether or not $\hat{\Omega}(\beta) \cap \Omega^{SN}$ is empty can be checked using a sum-of-squares program. This fact is formally stated in the following proposition.

Proposition 4.1: Let $\hat{\Omega}(\beta)$ be the certificate set (12). If there exist polynomials $V(\mu)$ and $r(\mu)$ and a constant $\beta > 0$ such that

$$a_{n-1}^2(\mu)(V(\mu) - \beta) + r(|\mu|)a_n(\mu) \text{ is SOS}, \quad (13)$$

then $\Omega^{SN} \cap \hat{\Omega}(\beta) = \emptyset$.

Proof: Verifying the condition $\Omega^{SN} \cap \hat{\Omega}(\beta) = \emptyset$ amounts to check the emptiness of the set

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

Using the positivstellensatz (p-satz) theorem [34, 35], the emptiness of this set is guaranteed by the existence of SOS polynomials $s_0, s_1$, polynomials $V(\mu), t(\mu)$ and constant $\beta > 0$ such that

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

Let $s_0 = 0, m = 1, s_1 = (V(\mu) - \beta)r(\mu)$. We have

$$s_1(V(\mu) - \beta) = (V(\mu) - \beta)[a_{n-1}^2(\mu - \beta) + r(\mu)a_n],$$

which implies the SOS condition in (13). Now consider any $\mu \in \Omega^{SN}$ for which the condition $a_n(\mu) = 0$ is satisfied. Upon substitution with the SOS condition in (13), we have

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

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

In a similar way, one can obtain an SOS condition for the non-existence of a Hopf bifurcation, which is stated in the following proposition.

Proposition 4.2: Let $\hat{\Omega}(\beta)$ be a certificate set (12). If there exist polynomials $V(\mu)$ and $r(\mu)$ and a real constant $\beta > 0$ such that

$$V(\mu) - \beta + r(\mu)\Delta_{n-1}(\mu) \text{ is SOS}, \quad (14)$$

then $\Omega^{H} \cap \hat{\Omega}(\beta) = \emptyset$.

Proof: Verifying the condition $\Omega^{H} \cap \hat{\Omega}(\beta) = \emptyset$ amounts to check the emptiness of the set

$$\{\mu | \Delta_{n-1} = 0, V(\mu) - \beta \neq 0, -(V(\mu) - \beta) \geq 0\}.$$ 

Using the p-satz theorem, this set is empty if there exist SOS polynomials $s_0$ and $s_1$, polynomials $V(\mu)$ and $t(\mu)$, and a constant $\beta > 0$ such that

$$s_0 - s_1(V(\mu) - \beta) + (V(\mu) - \beta)^{2m} + t(\mu)\Delta_{n-1} = 0.$$ 

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

$$s_1(V(\mu) - \beta) = (V(\mu) - \beta)[(V(\mu) - \beta) + r(\mu)\Delta_{n-1}],$$

which implies the SOS condition in (14). Now consider any $\mu \in \Omega^{H}$ for which the condition $\Delta_{n-1}(\mu) = 0$ is satisfied. Substitution to the SOS condition in (14) gives $V(\mu) > \beta$ which implies that any $\mu \in \Omega^{H}$ lies outside the level set defined by $V(\mu) \leq \beta$.

The SOS programs in Propositions 4.2 and 4.1 characterize those $\beta$ for which the associated certificate set $\hat{\Omega}(\beta)$ is bifurcation free. Clearly, if one were to identify the maximum value of $\beta$ for which, say, proposition 4.2 held, then this $\beta$ could be used to bound the minimum distance to bifurcation. In particular, let $\mu_0$ be an initially known parameter vector. Define the certificate function as $V(\mu) = \alpha(|\mu - \mu_0|)$ where $\alpha$ is class $K$, and let $\beta$ denotes the largest real constant for which, say, Proposition 4.2 holds. Then the distance-to-bifurcation, $\gamma$, can be bounded below as $\gamma = |\mu^* - \mu_0| \geq \alpha^{-\frac{1}{\beta}}(\beta)$. One obvious choice for $\alpha$ is to let it be $|\mu - \mu_0|$. This observation is formalized in the following proposition which is stated for the saddle node bifurcation condition in
Proposition 4.1. Clearly a similar result would hold for the Hopf bifurcation and the associated proposition is not stated due to space limitations.

Proposition 4.3: Consider system (3) and its Jacobian matrix defined in (7). Let $\mu^0$ be the initial parameters and let $\mu^*$ denotes the critical parameters at which a saddle node bifurcation occur. If there exists a constant $\beta > 0$, polynomials $\tilde{V} = |\mu^* - \mu^0|$ and $r(\mu)$ such that the following SOS program

$$\max \beta$$

s.t. $a_{n-1}^{\beta}(\mu)\tilde{V}(\mu) - r(\mu)an(\mu)$ is SOS,

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

Proof: From the proposition’s assumption, we know a saddle-node bifurcation exists, therefore the set $\Omega^{SN}$ is not empty. Since no bifurcation takes place at $\mu^0$, one can take the infimum of this set, say $\inf(\Omega^{SN})$. Note that the sets $\tilde{\Omega}(\beta)$ are compact sets, so there exists $\beta = \inf(\Omega^{SN})$ such that for any $\beta < \beta$ we know from Proposition 4.1 that no saddle node bifurcation occurs.

V. Example: Tritrophic Foodweb

This example is used to illustrate the complexity of food chain models due to the presence of many parameters. It also describes how different mechanism can lead to bifurcations in food webs of aquatic eco-systems. This particular example examines a tri-level food chain [36] and shows that the proposed solution to the distance-to-bifurcation problem identifies a smaller distance to bifurcation than competing bifurcation tools such as XPPAUT [37]. This is because these competing tools are usually restricted to only one or two-parameter bifurcations. The example in this section shows that the correlated variation in several system rate constants can lead to a significantly smaller distance to bifurcation than was identified using XPPAUT to identify 1-parameter bifurcation points.

We consider the following tritrophic food chain model from [36].

$$\begin{align*}
\dot{X}_1 &= X_1 (1 - X_1) - k_1 X_1 X_2 \frac{1}{1 + X_1}, \quad X_1(0) = x_{10}, \\
\dot{X}_2 &= \frac{k_1 X_1 X_2}{1 + X_1} - k_2 X_2 X_3 - k_3 X_2, \quad X_2(0) = x_{20}, \\
\dot{X}_3 &= k_2 X_2 X_3 - k_4 X_3, \quad X_3(0) = x_{30},
\end{align*}$$

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. Parameter $k_1 (k_2)$ describes the consumption rate of primary consumer (top predator) on primary producer (primary consumer), whereas $k_3 (k_4)$ denote the death rate of primary consumer (top predator). Introducing a time scaling $d\tau = (1 + X_1)dt$ and defining $dX_i/d\tau = \dot{x}_i$, an equivalent model of the above tritrophic food chain system is given by

$$\begin{align*}
\dot{x}_1 &= x_1 (1 - x_1) (1 + x_1) - k_1 x_1 x_2, \\
\dot{x}_2 &= k_1 x_1 x_2 - k_2 x_2 x_3 (1 + x_1) - k_3 x_2 (1 + x_1), \\
\dot{x}_3 &= k_2 x_2 x_3 (1 + x_1) - k_4 x_3 (1 + x_1),
\end{align*}$$

with initial condition $x_0 = (x_{10}, x_{20}, x_{30})^T$. Population limit cycles or extinction are often related to the presence of a bifurcation. In the following, we use the proposed method to search for critical parameters that induce a bifurcation.

The system’s kinetic realization has a matrix $N$ and vector $v(x, k)$ of the following form,

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

$$v = [x_1, x_1^3, k_1 x_1 x_2, k_2 x_2 x_3, k_3 x_2, k_3 x_1 x_2, k_4 x_3 k_4 x_1 x_3]^T.$$

The matrix $Z$ which satisfy $v(x, k) = \text{diag}(k) x^Z$ is

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

Due to space limitations, we only state the results for the state equilibrium parametrization. A detailed example of this computation can be found in [38]. As discussed above, the computation of this parameterization has two parts: the parameterization of equilibrium fluxes $v^*(\lambda)$ and then the computation of the Gröbner basis for the toric ideal. CellNetAnalyzer [27] identified seven extreme generators to form the convex cone (5) and the associated parameterization of the equilibrium fluxes are given by

$$v^*(\lambda) = \{\Sigma_{i=1}^7 \lambda_1, \lambda_3, \Sigma_{i=1}^7 \lambda_1 - 3\lambda_3, \lambda_4 + \lambda_6, \lambda_5 + \lambda_7, \lambda_1, \lambda_2, \lambda_6 + \lambda_7, \lambda_4 + \lambda_5\}.$$ 

A Gröbner basis for the toric ideal was computed using SINGULAR [31] and is given by

$$v^*(k) = \{v_6 v_9 - v_7 v_8, k_3 v_3 - k_1 v_7, k_3 k_4 v_4 - k_2 v_6 v_8, v_2 v_6^3 - v_7^3, v_5 v_8 - v_4 v_9\}.$$

The intersection of these two fluxes representation gives the following relation between the system and the convex parameters.

$$0 = \lambda_3 \lambda_1^3 - \lambda_2^3,$$

$$0 = k_1 \lambda_2 - k_3 (\Sigma_{i=1}^7 \lambda_1 - \lambda_3),$$

$$0 = \lambda_1 (\lambda_4 + \lambda_5) - \lambda_2 (\lambda_6 + \lambda_7),$$

$$0 = k_3 k_4 (\lambda_4 + \lambda_6) - k_2 k_1 (\lambda_5 + \lambda_7),$$

$$0 = (\lambda_5 + \lambda_7) (\lambda_6 + \lambda_7) - (\lambda_4 + \lambda_5) (\lambda_4 + \lambda_6).$$

Using this relation and by the fact that $v^* = \text{diag}(k) x^Z$, the parameterized state equilibrium is given by

$$x_1^* = \Sigma_{i=1}^7 \lambda_1, \quad x_2^* = \lambda_1 / k_3, \quad x_3^* = (\lambda_6 + \lambda_7) / k_4.$$
We now use this parameterization to characterize the system’s Jacobian matrix (7). Letting $h_1 = 1/x^*$, the Jacobian is given by

$$
J = \begin{bmatrix}
-2h_1\lambda_3 & -h_2(\Sigma_i^3 - \lambda_i) & 0 \\
-h_1(\Sigma_i^1 - \lambda_i) & 0 & -h_2\Sigma_i^3 \\
-h_1(\lambda_i - \lambda_7) & h_2\Sigma_i^3 & 0
\end{bmatrix}
$$

with characteristic polynomial \( p(s) = s^4 + a_1s^3 + a_2s^2 + a_3s + a_4 \). One can verify that \( a_1, a_2, a_3 \) are positive since \( h_i, k_j \) are always positive. The last coefficient \( a_4 \) has the form

$$
a_4 = \lambda_4^2 - \lambda_7^2 + (\lambda_4 - \lambda_7)\Sigma_i(1,2,5,6)\lambda_i + 2\lambda_3\Sigma_i^7 = 0
$$

which consists of both positive and negative terms. The coefficient \( a_4 \), therefore, may be zero from appropriate choices of the system parameters. Proposition 4.3 was used to compute the closest bifurcation \( \gamma \) with decision variables \( \mu = \lambda_i (i = 1, \ldots, 7) \), for a specific choice of initial parameter vector \( k^0 \). Note that the corresponding system parameters \( k_i \) can always be recovered from known \( \lambda \) and vice versa.

Let the initial parameter be \( k^0 = (0.5, 0.2, 0.01, 0.3) \) that has a stable equilibrium at \( x^*_a = (0.5, 1.5, 0.783) \). The associated \( \mu \) parameter vector is then given by \( \mu^0 = (0.15, 0.066, 0.085, 0.12, 0.12, 0.12, 0.12, 0.12) \). From the SOS-TOOLS, we obtained a lower bound on the distance to bifurcation of \( \gamma = 0.0032 \) which corresponds to critical parameter \( k^* = (0.51, 0.205, 0.05, 0.4) \). This particular parameter vector, in fact, was shown to result in a bifurcation through simulation analysis. On the other hand, a one dimensional bifurcation analysis using XPPAUT [37] gives the distance \( \gamma_{FPF} = 0.0246 \) which corresponds to parameter \( k_3 = 0.1667. \) This example shows that correlated variations in all system parameters can lead to a much smaller distance to bifurcation \( (\gamma = 0.0032) \) than was obtained through a 1-parameter bifurcation analysis.

VI. Final Comments

This paper used sum-of-squares relaxations to obtain a lower bound on the minimum distance-to-bifurcation in non-negative systems that had kinetic realizations. Many real-life systems have such realizations and the value of this approach is it allows one to recast the distance-to-bifurcation problem as a sum-of-squares program that can be efficiently solved using semidefinite programming codes. The method was demonstrated on a tritrophic food web and the example showed that the proposed approach was able to detect how correlated variations in system rate constants could lead to smaller distance-to-bifurcations than are usually found with conventional 1 or 2 parameter bifurcation tools. While the paper focused on applying these methods to eco-systems, we have also applied them to signaling pathways in cellular systems and voltage collapse in electrical power grids. The proposed methods represents a powerful “cyber” tool for studying how sensitive a complex nonlinear systems may be to environmental parameter changes.

References


