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Using Elementary Flux Modes to Estimate the Distance to Regime Shifts in Kinetic Systems ⋆

M.D. Lemmon * **T.A. Tamba** *

* *Dept. of Electrical Engineering, University of Notre Dame, Notre Dame, IN 46556, USA (e-mail: lemmon@nd.edu).*

Abstract: This paper studies *regime shifts* in dynamical systems with *kinetic realizations*. A regime shift occurs when small external disturbances shift the system's state from a *nominal* to an *alternative* qualitative behavior. Kinetic systems are dynamical systems found in biological networks that are defined with respect to a directed graph modeling mass/energy transport. This paper estimates the *distance-to-regime-shift* (DTRS) using robust stability concepts. A novel feature of the work is its parameterization of the network using *elementary flux modes* (EFM). EFMs represent fundamental pathways governing the fate of species in the network. The advantage of this parameterization is that the linearized system can be written as an affine parameter dependent (APD) system. The robust stability of APD systems can be checked through a linear matrix inequality (LMI) feasibility problem. The DTRS analysis, therefore, is computationally tractable since there exist efficient solvers for such LMI problems. This is demonstrated for an oscillator system that has been used to study the robustness of biochemical systems.

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1. INTRODUCTION

A variety of natural and man-made dynamical processes provide essential goods and services to humanity. There is a growing concern that these processes may not be *resilient* to stressors such as climate change and globalization. Evidence of this concern is found in the recent national climate assessment of Karl et al. (2008) that warns of more frequent storms disrupting electrical power delivery. Another example is found in the recent closure of Toledo's water system arising from toxic algae blooms whose occurrence is exacerbated by increased storm run-off. These concerns suggest we need better ways to predict and manage societal disruptions triggered by external stressors.

One important type of disruption is a *regime shift*. Regime shifts occur when small perturbations or disturbances shift the system's state away from a *nominal* to an *alternative* qualitative behavior. The term "regime shift" has its origins in the ecological systems community. Examples of regime shifts in ecological systems may be found in Folke et al. (2004). The concept may also be illustrated in Figure 1. In this figure a given system's function is shown on the y-axis and the strength of the external stressor (disturbance) is shown on the x-axis. For low intensity stressors, the system function stays within the nominal range shown in Figure 1. But when the strength of that stressor grows beyond a certain threshold the system function will decline rapidly, thereby signaling the occurrence of a *regime shift* in the system.

Gallopín (2006) describes regime shift resilience with respect to three dimensions; 1) vulnerability, 2) recovery, or 3) adaptive capacity. These three dimensions are illustrated in Figure 1. In this figure a system's regime shift vulnerability is characterized by the strength of the stressor triggering an abrupt decline in system function. Recovery refers to the fact that catastrophic shifts will eventually happen and develops interventions to recover lost system functionality after a shift has occurred. This dimension is measured by the time and cost it takes to force a shift between two competing regimes. Finally, adaptive capacity measures the ability of a system to reduce its vulnerability and strengthen its recovery. In particular this adaptation may be seen as the system's ability to shift its function curve to the right as shown in Figure 1. Of these three problems, this paper focuses on assessing a system's vulnerability to regime shifts.

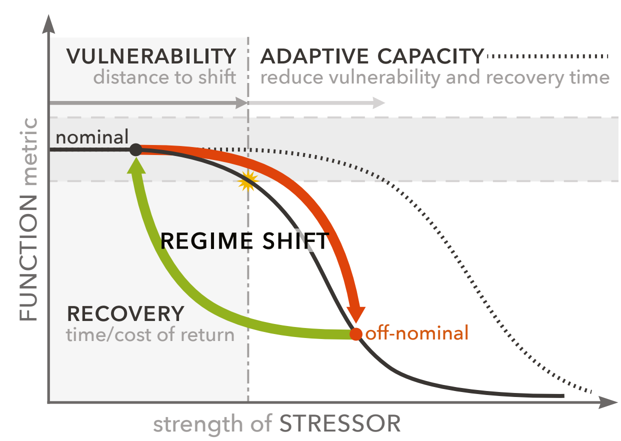

Fig. 1. Dimensions for Resilience: The system function (black line) decreases rapidly after a threshold characterizing the system's *vulnerability* to a regime shift. Resilience may be measured by the cost and effort needed to recover from a shift as well as the *capacity* to shift the system function curve to the right (dotted line).

This paper views that vulnerability issue as a robust stability problem. Regime shifts occur in dynamical systems when the system's state shifts from the neighborhood of a *nominal*

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equilibrium to that of an *alternative* equilibrium. Since global dynamic behavior is often determined by the stability types of all of the system equilibria; a change in the stability type (i.e. stable to unstable node) is a necessary condition for such a regime shift. Assessing a system's vulnerability to such shifts, therefore, may be estimated by determining the largest parameter set for which a change in stability type is guaranteed *not* to occur. Stated in this way the problem of estimating a system's regime shift vulnerability is recast as a robust stability problem.

This paper solves this problem for the class of so-called *kinetic systems*. A kinetic system is a nonnegative polynomial system defined over a directed graph modeling conserved flows of energy or mass. These system realizations often occur in modeling chemical reaction networks with mass action kinetics. While this type of system has its origins in chemical reaction networks, the models are very general in that a *kinetic realization* can be constructed for just about any dynamical process satisfying a conservation law. The main modeling requirement is that the system dynamics be finitely generated over a suitable algebra of functions. These conditions are satisfied by networked dynamical systems such as traffic flows, electric power systems, ecosystems, and cellular regulatory networks.

Prior work has studied the robust stability of kinetic systems using a variety of tools. It has been treated as an inverse bifurcation problem that seeks the smallest parameter variation triggering a local bifurcation. Dobson and Lu (1993), for example, used numerical continuation methods to solve the inverse bifurcation problem in electrical power systems. Another approach uses convex optimization to search for functions certifying the robust stability of the system. Waldherr and Allgöwer (2011) used this approach to search for certificates over a function space spanned by Handelman polynomials. Tamba and Lemmon (2014) used a similar approach that used semidefinite programming to search for a valid certificate over the space of sum-of-squares (SoS) polynomials. Other work in Motee et al. (2012) used M-matrix conditions to evaluate robust stability in biochemical networks.

A major limitation of this prior work is that the methods are often computationally intractable for moderately sized problems. Numerical continuation methods are limited to systems with no more than 2-3 parameters. Certificate methods based on Handelman polynomials suffer from the large number of basis polynomials needed to capture the constraint. Similar problems are found with the use of SoS polynomials due to the state of existing semidefinite program (SDP) solvers. Finally, checking to see if a system is an M-matrix can lead to high order semi-algebraic constraints whose positive definiteness is difficult to certify.

The approach adopted in this paper addresses the computationally intractability of the kinetic system's robust stability problem by reparametrizing the system with respect to its *elementary flux modes* (EFM). Elementary flux modes are the extreme rays that generate a convex polytopic cone containing all *equilibrium fluxes* of the system. Clarke (1980) used EFMs to study reaction network stability. Schuster and Hilgetag (1994) observed that *elementary flux modes* (EFM) form fundamental pathways generating the reaction network's dynamics. Conradi et al. (2007) used this fact to suggest a subnetwork analysis for kinetic systems.

This paper shows that parameterizing the kinetic system in terms of the EFM activity levels leads to a linear affine parameter dependent (APD) description of the system's Jacobian matrix. Barmish and DeMarco (1986) showed that the robust stability problem for APD systems can be solved by finding a parameter-dependent Lyapunov function. When the parameter uncertainties lie within a polytopic set, Gahinet et al. (1996) cast this search as a system of linear matrix inequalities (LMI). Since LMIs can be efficiently solved using tools like those described in Gahinet et al. (1994), it is possible to efficiently solve the kinetic system's robust stability problem. This paper demonstrates the feasibility of that approach on a biochemical oscillator system used in Ma and Iglesias (2002) to quantify the robustness of biochemical networks. This is a moderately sized system with 7 states and 14 parameters. We use this system to demonstrate that the use of EFM parameters leads to a computationally tractable method for evaluating the system's vulnerability to regime shifts.

Notation: Component-wise division and multiplication of vectors $x, y \in \mathbb{R}^n$ are denoted as x/y and xy, respectively. A polynomial, $p(x; k)$, with variables $x = \{x_1, \ldots, x_n\}$ and parameters $k = \{k_1, \ldots, k_m\}$ is a formal series

$$p(x; k) = \sum_{j=1}^{m} \pm k_j \prod_{\ell=1}^{n} x_\ell^{y_{j\ell}} \tag{1}$$

where $y_{j\ell}$ are integers for $j = 1, 2, \ldots, m$ and $\ell = 1, 2 \ldots, n$. The set of all such polynomials whose parameters take values in the real field is denoted as $\mathbb{R}(k)[x]$. The n-dimensional row vector $\overline{y}_j = [y_{j1}, y_{j2}, \ldots, y_{jn}]$ for $j = 1, 2, \ldots, n$ is called a *multi-index* and $x^{[\overline{y}_j]}$ denotes the monomial generated by multi-index $\overline{y}_j$. Let Y be an integer matrix whose rows are the m monomial terms in $p(x; k)$, then the m-vector of monomials in $p(x; k)$ is written in multi-index notation as $x^{[Y]}$.

A labeled directed graph, $G = (V, E, L)$ is a triple consisting of a set V of n vertices, a set L of m labels, and a set $E \subset V \times V \times L$ of p labeled edges. For an edge, $e = (v, w, k)$, we refer to $v \in V$ as the edge's initial vertex, $w \in V$ as the edge's terminal vertex, and $k \in L$ as the edge's label. We define graph G's incidence matrix B where the matrix' ijth element, b_{ij} is 1 if vertex i is the initial vertex of edge j, is -1 if vertex i is the terminal vertex of edge j, and is zero otherwise. We introduce a *reduced incidence matrix*, $\tilde{B}$, whose elements $\tilde{b}_{ij} = b_{ij}$ if $b_{ij} = -1$ and is zero otherwise.

2. KINETIC SYSTEMS

Consider a polynomial system whose n-dimensional state trajectory $x(\cdot) : \mathbb{R}_{\geq 0} \to \mathbb{R}^n$ satisfies $\dot{x} = f(x; k)$ with initial condition $x(0) = x_0$. This system is *polynomial* if $f(x; k) \in \mathbb{R}(k)[x]$. The polynomial vector $f(x; k)$ for $k \in \mathbb{R}^m$ is *essentially nonnegative* if $f_i(x; k) \geq 0$ for all $i = 1, 2, \ldots, n$ and all $x \geq 0$ for which $x_i = 0$. The system will be said to be *nonnegative* if the nonnegative real cone, $\mathbb{R}^n_{\geq 0}$, is positively f-invariant. Haddad and Chellaboina (2005) show that a polynomial system is nonnegative if and only if $f(x; k)$ is essentially nonnegative.

Consider an n-dimensional nonnegative polynomial system, $\dot{x} = f(x; k)$. This system has a *kinetic realization* if there exists a labeled directed graph, $G = (V, E, L)$ where V is a finite set of q multi-indices of length n, L is a set of m parameters, and $E \subset V \times V \times L$ is a set of p labeled edges such that

$$\dot{x} = f(x; k) = Y^T B I_k x^{[Y]} \tag{2}$$

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