

Forecasting Regime Shifts in Natural and Man-made Infrastructure

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Motivation - why do this?

- Human society relies on many natural and man-made processes to deliver a *consistent* level of essential goods and services.
 - Ecosystem services - clean air, water, food, and fiber
 - Man-made systems - power, water, and traffic networks
- These processes are *infrastructure* systems since they form the basis of a civil society and disruptions to infrastructure service delivery has a strong impact on public health and welfare.
- 2014 National Climate Assessment warns of climate change's potential to disrupt those services, with negative impact on public health and welfare.
- One kind of infrastructure disruption is a *regime shift*.

What is a Regime Shift?

- A regime shift occurs when a system shifts its state trajectory from a *nominal* operating point to an *alternative* operating point for an extended period of time.
- Example is cultural eutrophication of aquatic ecosystem



- Nutrient enrichment from human sources triggers a toxic algae bloom.
- Negative impacts include reduced water quality, fish kills, toxic algae blooms, reduced biodiversity

Regime Shift Mechanisms in Aquatic Ecosystems

- Regime shifts occur in response to the disturbance of a system's internal parameters and can be categorized with regard to disturbance time-scale
 - Fast disturbances that are impulsive in nature give rise to *shock-induced* shifts.
 - Slow disturbances give rise to *bifurcation-induced* shifts

P = phosphorus in water column

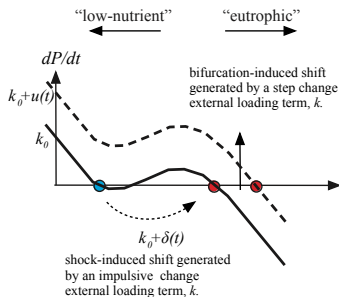
u = rate of external nutrient loading

α = rate at which P sorbs to sediment

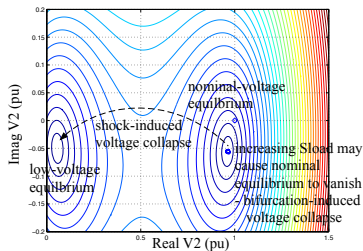
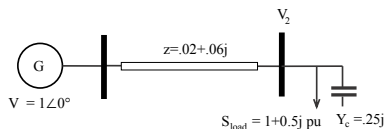
ρ = rate at which sediment P desorbs

$$\frac{dP}{dt} = \underbrace{k(t)}_{\text{external load}} - \underbrace{\alpha P}_{\text{sink term}} + \underbrace{\frac{\rho P^3}{\theta^3 + P^3}}_{\text{internal load}}$$

source terms



Regime Shift Mechanisms in Power Systems



- The same mechanisms trigger voltage collapse in two bus system with two equilibria
- Voltage collapse occurs if increase in demand causes nominal voltage equilibrium to vanish
- Voltage collapse occurs if fault causes voltage to jump into low voltage RoA

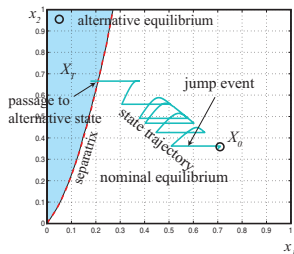
Shock-induced Shifts as First Passage Time Problem

We want to bound the likelihood of a shock-induced shift for

$$dx(t) = f(x(t))dt + dJ(t)$$

where $J(t)$ is a shot noise process.

If the initial state is at nominal equilibrium, x_0 , and X_T is the ROA of the alternative equilibrium, then the *first passage time* is the first time the system state $x(t; x_0)$ enters X_T . This time is a random variable.

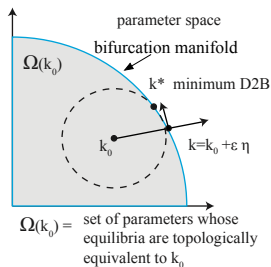


The distribution of this *first passage time* (FPT) characterizes the likelihood of a shock-induced regime shift

Distance to Bifurcation-induced Shifts (D2B)

We want to determine the range of parameters about a nominal parameter k_0 for which system $\dot{x} = f(x; k)$ does not have a bifurcation.

- A parameter, k , is *topologically equivalent* to the nominal parameter if the flows of their equilibria can be smoothly mapped into each other.
- *Bifurcation* occurs for a system that is *not* topologically equivalent to the nominal system.



The minimum *distance-to-bifurcation* (D2B) is the distance to the bifurcating system that is closest to k_0 . This distance characterizes sensitivity to bifurcation-induced shifts.

Model-based Method for Regime Shift Prediction

- We are using a common analysis framework to solve both the FPT and D2B problems
- The benefits of the proposed method are that it
 - obtains *bounds* on parameters for which no regime shifts occur.
 - obtains tighter bounds than other approaches
 - analysis can be done using existing computational tools
- In exchange for these benefits, we need to *realize* the process as a *polynomial system*
- For such polynomial realizations, one can use barrier certificates and concepts from algebraic geometry to recast the FPT/D2B problem as a polynomial optimization problem
- Approximations of this problem's solution are then computed using a sequence (hierarchy) of semidefinite programming (SDP) or linear programming (LP) relaxations.

Polynomial System Realizations

- A polynomial realizations does not mean the system is polynomial.
- Consider a system whose original state \tilde{x} satisfies

$$\dot{\tilde{x}} = F(\tilde{x}, k)$$

where F is a smooth vector field with system states \tilde{x} and parameters k .

- Introduce a diffeomorphism $T : \mathbb{R}^{\tilde{n}} \rightarrow \mathbb{R}^n$ and define the new state $x = T\tilde{x}$.
- The original system has a polynomial realization if one can find a diffeomorphism T such that

$$\dot{x} = T\dot{\tilde{x}} = TF(T^{-1}(x); k) = f(x; k)$$

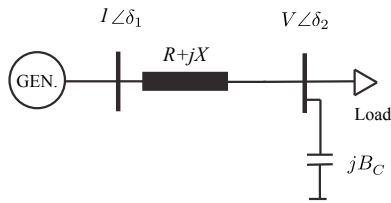
in which f is an element of the polynomial ring $\mathbb{R}(k)[x]$ with variables x and real coefficients k

How Restrictive are Polynomial Realizations?

- Polynomial realizations were studied back in the 1980's which established necessary and sufficient conditions for the existence of such realizations.
- Primary result in [Bartosiewicz, Minimal polynomial realizations, *Mathematics of Control, Signals, and Systems*, 1988] made use of algebraic characterizations of observability and provided a constructive approach.
- So in many cases, even a system that is not polynomial may have a polynomial realization with a clever variable substitution.
- Even if this cannot be done, one can still approximate any smooth vector field on a compact domain using polynomials.

Polynomial Realization of Two bus System

Introduce the variable transformation $x = \cos \delta$ and $y = \sin \delta$ and add ODE's for \dot{x} and \dot{y}



$$\dot{\omega} = \frac{1}{M} [P_m - P_{e1}(\delta, V) - D_G \omega]$$

$$\dot{\delta} = \omega - \frac{1}{D_L} [P_{e2}(\delta, V) - P_d]$$

$$\dot{V} = \frac{1}{\tau} [Q_e(\delta, V) - Q_d]$$

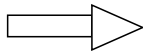
$$P_{e1} = G - V(G \cos \delta - B \sin \delta)$$

$$P_{e2} = -V^2 G + V(G \cos \delta + B \sin \delta)$$

$$Q_e = -V^2 B - V(G \sin \delta - B \cos \delta)$$

$$x = \cos \delta$$

$$y = \sin \delta$$



$$\dot{\omega} = \frac{1}{M} [P_m - (G - V(Gx - By)) - D_G \omega]$$

$$\dot{\delta} = \omega - \frac{1}{D_L} [-V^2 G + V(Gx + By) - P_d]$$

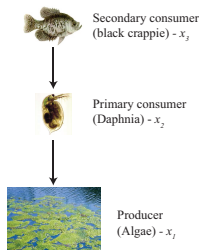
$$\dot{V} = \frac{1}{\tau} [-V^2 B - V(Gy - Bx) - Q_d]$$

$$\dot{x} = -y \left[\omega - \frac{1}{D_L} [-V^2 G + V(Gx + By) - P_d] \right]$$

$$\dot{y} = x \left[\omega - \frac{1}{D_L} [-V^2 G + V(Gx + By) - P_d] \right]$$

Polynomial Realization of Foodweb

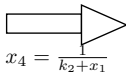
- Three level aquatic food web consisting of producers (x_1), primary consumers (x_2) and secondary consumers (x_3).
- Introduce new variable $x_4 = \frac{1}{k_2+x_1}$ and add ODE for the new state.



$$\dot{x}_1 = x_1(1-x_1) - \frac{k_1 x_1 x_2}{k_2 + x_1}$$

$$\dot{x}_2 = \frac{k_3 x_1 x_2}{k_2 + x_1} - k_4 x_2 x_3 - k_5 x_2$$

$$\dot{x}_3 = k_6 x_2 x_3 - k_7 x_3$$



$$\dot{x}_1 = x_1(1-x_1) - k_1 x_1 x_2 x_4$$

$$\dot{x}_2 = k_3 x_1 x_2 x_4 - k_4 x_2 x_3 - k_5 x_2$$

$$\dot{x}_3 = k_6 x_2 x_3 - k_7 x_3$$

$$\dot{x}_4 = -x_4^2 [x_1(1-x_1) - k_1 x_1 x_2 x_4]$$

Barrier Certificates

- When the system is polynomial we can use *Certificates* to verify system theoretic property such as stability, reachability, or safety.
- Introduce a *test set* whose emptiness verifies the property of interest
- The test set's emptiness is verified using the *positivstellensatz* (p-satz) theorem for the semi-algebraic set

$$\Omega = \{x \in \mathbb{R}^n : F_i(x) \geq 0 \text{ and } G_j(x) = 0 \text{ for all } i, j\}$$

The set Ω is empty if and only if there are polynomials F in the cone generated by $\{F_i\}$ and G in the ideal generated by $\{G_j\}$ such that $F + G + 1 = 0$.

- The existence of this function is taken as a *certificate* of the emptiness of Ω and hence verifies the system property.

Barrier Certificate for Asymptotic Stability

- Let the property of interest be that *the equilibrium is asymptotically stable with a specified rate of convergence slower than β* .
- This property has a Lyapunov characterization in which we seek a *certificate* $V(x)$ such that $V(x) \geq 0$ and $-\beta V(x) > \dot{V}(x)$. These inequalities form the test set to which the p-satz theorem is applied. If a certificate is found then the convergence rate must be slower than β .
- Apply the p-satz as an *oracle machine* that drives a bisection search for the optimal β .
- Barrier certificates can therefore be used to *optimize* the desired system theoretic property.

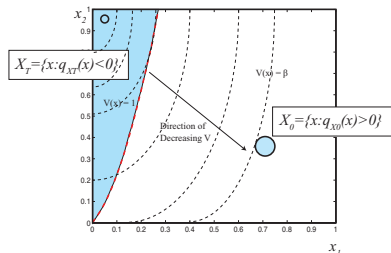
Certificates for Shock-induced Regime Shifts

- For the FPT problem the system property is that a state trajectory starting at x_0 (nominal equilibrium) leaves the nominal RoA within a deadline T and a probability that is less than $1/\gamma$. (*Stochastic Reachability*)
- The certificate whose existence verifies this property is a polynomial function V such that $V(x(0)) = 1$, $V(x(t)) < \gamma$ for $t \in [0, T]$ and $\mathcal{L}V < 0$.
- The condition that system's generator satisfy $\mathcal{L}V < 0$ ensures $V(x(t))$ is a super-martingale so that

$$\mathbb{P} \{V(x(t)) > \gamma : x_0\} < \frac{1}{\gamma}$$

This provides a bound on the probability of leaving the nominal ROA by deadline T .

Solving FPT Problem using SOS Relaxations



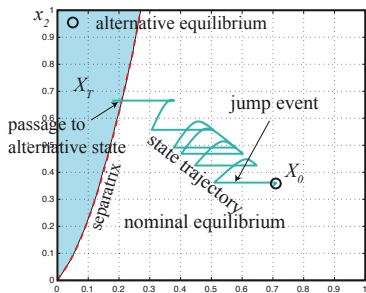
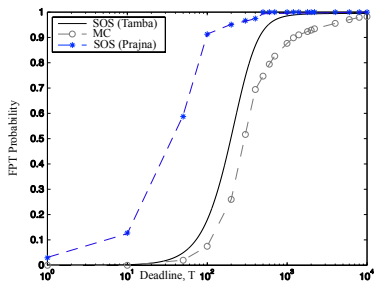
When the system equations and barrier certificates are polynomial functions, then SOS relaxations can be used to find the best barrier certificate.

We assume the sets X_0 and X_T can be specified by polynomials $q_{X_0}(x, t)$ and $q_{X_T}(x, t)$. The associated SOS program is then

$$\begin{aligned}
 &\text{minimize:} && \beta \\
 &\text{w.r.t.} && \text{polynomials, } V(t, x), p_X(x, t), p_{X_T}(x, t), p_{X_0}(x, t), \text{ and constant } \beta \text{ and } \epsilon \\
 &\text{subject to:} && -V(t, x) - \beta - p_{X_0}(x, t)q_{X_0}(x, t) \text{ is SOS} \\
 &&& V(t, x) - 1 - p_{X_T}(x, t)q_{X_T}(x, t) \text{ is SOS} \\
 &&& V(t, x) - p_X(x, t)q_X(x, t) - \epsilon \text{ is SOS} \\
 &&& -\frac{\partial V}{\partial t} + \mathcal{L}^*V(t, x) - p_X(t, x)q_X(t, x) - \epsilon \text{ is SOS}
 \end{aligned}$$

Improvements to the Approach

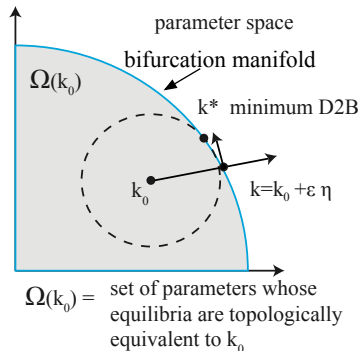
- Preceding approach [Prajna2007framework] assumed Brownian diffusions. We've extended this to jump processes.
- The super-martingale condition in [Prajna2007framework] was improved to letting $\mathcal{L}V(x) < -\alpha V(x) + \beta(t)$ to obtain tighter upper bound on FPT distribution.



Prior Work on D2B Problem

Early work on D2B problem was used to predict voltage collapse in simple power systems

This work used numerical continuation methods to search the bifurcation manifold for the minimum D2B. The result was a locally optimal solution that only provided an upper bound on the minimum D2B.

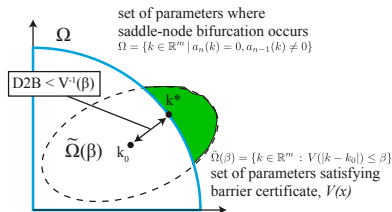


Moreover, the computational complexity of most continuation software limits us to problems with only 2-3 parameters.

Certificate for Bifurcation-induced Shift

- Certificate methods solve the D2B problem in the parameter space, rather than the state space.

Given a nominal parameter, k_0 , The test set consists of those parameters which are *not* topologically equivalent to k_0 and those parameters that are within a distance β of k_0 .



- Finding a certificate verifies that minimum D2B is greater than β . Use p-satz as an oracle machine to determine greatest lower bound on D2B.

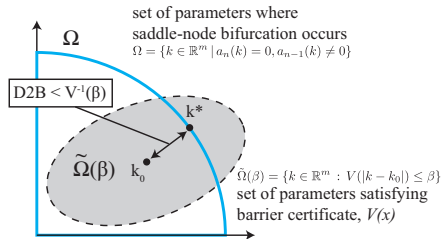
Solving the D2B Problem using SOS Relaxations

Emptiness of Ω is verified using a sum-of-squares (SOS) relaxation ¹.

In particular, consider $\beta > 0$ and $V \in \mathcal{K}$ such that

$$\tilde{\Omega}(\beta) = \{k : V(|k - k_0|) \leq \beta\}$$

For a given $\beta > 0$, the distance to bifurcation is less than $V^{-1}(\beta)$ if $\tilde{\Omega}(\beta) \cap \Omega \neq \emptyset$.



The SOS-relaxation searches for the largest β such that $\tilde{\Omega}(\beta) \cap \Omega = \emptyset$.

maximize: β

such that: $a_{n-1}^2(k)(V(|k - k_0|) - \beta) + r(k)a_n(k)$ is SOS

¹Parrilo, Semidefinite programming relaxations for semi-algebraic problems, Mathematical programming, 96(2):293-320, 2003

Voltage Collapse Example

- The polynomial equations characterizing the bifurcation point of two-bus system

$$\begin{aligned}0 &= -GV^2 + GVy + BVx - P_d \\0 &= -BV^2(B - G)Vy - Q_d \\0 &= G^2 + B^2 - 2B^2Vx - 2G^2Vy \\0 &= x^2 + y^2 - 1\end{aligned}$$

- This system is generated by a single polynomial

$$p(P_d) = \beta_1 + \beta_2 P_d + \beta_3 P_d^2$$

- The D2B problem is now to find an SOS polynomial $r(P_d)$ that

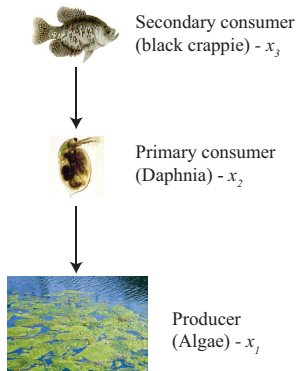
$$\begin{aligned}\text{maximize:} & \quad \gamma \\ \text{subject that:} & \quad (P_d - P_d^0)^2 + (P_d/4 - Q_d^0)^2 - \gamma + r(P_d)p(P_d)\end{aligned}$$

Regime Shifts in Aquatic Foodwebs

This approach can also be used on ecosystems. The following foodweb exhibits a Hopf bifurcation².

Three-level aquatic foodweb consisting of producers (x_1), primary consumers, (x_2), and secondary consumers (x_3).

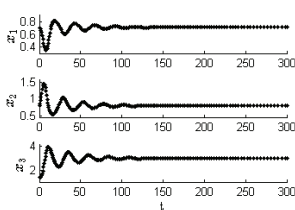
$$\begin{aligned}\dot{x}_1 &= x_1(1 - x_1) - \frac{k_1 x_1 x_2}{k_2 + x_1} \\ \dot{x}_2 &= \frac{k_3 x_1 x_2}{k_2 + x_1} - k_4 x_2 x_3 - k_5 x_2 \\ \dot{x}_3 &= k_6 x_2 x_3 - k_7 x_3\end{aligned}$$



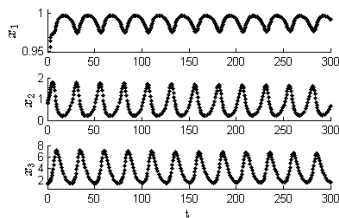
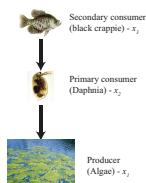
²A. Hastings, Chaos in three species food chain, Ecology, 72(3), 1991

Tritrophic Foodweb Example - cont'd

Foodweb with Stable Equilibrium



Hopf Bifurcation and Limit Cycle



- For this example, we compute a minimum D2B of $\boxed{0.0032}$.
- It is interesting to compare this to results obtained using a traditional bifurcation tool, XPAAUT ³,
- XPAAUT solves D2B problem for a single parameter at a time. It obtains a minimum D2B of $\boxed{0.1667}$ for parameter k_3 .
- We find greater sensitivity because we search over all parameters.

³Ermentrout, Sim. , analyzing, and animating dyn. sys., SIAM, 2002.

Some Tricks of the Trade

- The algebraic conditions for a local bifurcation require a characterization of the Jacobian matrix *as a function of k* .
 - Compute the solution to the polynomial system $0 = f(x; k)$ using Gröbner basis methods that are *doubly exponential* w.r.t variables
 - Trick is to project this system into a higher dimensional space in which we solve a system of *binomial* equations and then compute Gröbner basis for resulting *toric* ideal.
- Solving a polynomial optimization problem is *NP-hard*
 - We often use a sequence of semidefinite programming (SDP) relaxations to compute an approximation of the original problem.
 - The release of SOSStool provides a Matlab I/F for using SDP relaxations. These tools represent the certificate as a *sum-of-squares* (SOS) polynomial. But there are limitations on problem size.
 - Trick is to use LP relaxations based on Handelman or Bernstein polynomials

Benefits of Proposed Approach

- We've introduced a model-based approach for regime shift prediction.
- The approach assumes the process can be realized as a polynomial system
- Certificates allow us to recast problem as a polynomial optimization problem.
- The benefits of the approach are
 - Tighter bounds on the time or distance to regime shift
 - Lower bounds on the D2B represent a guaranteed region of stability
 - Computational tools exist to automate the solution.

Future Research Directions

- System Identification of Polynomial Realizations
- Construction of Local Regime shift Indices
- Computational Issues of Certificate Methods
- Prediction of Cascading Regime shifts (failures)
- Moving from Forecasting to Management
- Tool Development
- Evaluation Testbed in Aquatic Ecosystems and Power Systems

Formulation of the D2B Test Set

- Algebraic geometric methods allow us to express the bifurcation eigenvalue condition as a function of the parameters only.
- Let Ω denote the set of system parameters, k , for which a bifurcation (saddle-node) occurs. This set has the form ⁴

$$\Omega = \{k \in \mathbb{R}^m \mid a_n(k) = 0, a_{n-1}(k) \neq 0\}$$

where $a_n(k)$ and $a_{n-1}(k)$ are algebraic expressions for the coefficients in the Jacobian matrix' characteristic polynomial.

- One can therefore conclude that the system will not have a bifurcation if Ω is empty.

⁴Tamba et al., The Distance-to-Bifurcation Problem in Non-negative Dynamical Systems with Kinetic Realizations, IEEE Conf. on Control and Automation, 2014

Solving the D2B Problem for Hopf Bifurcation

- A necessary condition for a Hopf bifurcation is that the Jacobian's Hurwitz Determinant $\Delta_{n-1} = 0$.
- An algebraic expression for Δ_{n-1} can be determined directly from the system's Jacobian matrix,

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

- We can then use the p-satz theorem to construct an SOS program determining the minimum D2B,

$$\begin{aligned} & \text{maximize:} && \beta \\ & \text{subject to:} && V(\lambda, k) - \beta + r(\lambda, k)\Delta_{n-1}(\lambda, k) \text{ is SOS} \end{aligned}$$