CHAPTER 3

Bifurcation Induced Regime Shifts

Bifurcation-induced regime shifts occur when a perturbation in the system parameters changes the topology of the basic sets comprising the system regimes. A nominal system's susceptibility to a bifurcation-induced regime shift can be measured by the distance-to-bifurcation or D2B; namely the smallest parameter perturbation that triggers a shift in the topology of the basic sets. The D2B can therefore play a critical role in developing conservation policies that reduce the likelihood of an impending regime shift.

This chapter presents a method for computing bounds on a consumer-resource system's distance to a *local bifurcation* of its equilibria. In particular, we show that *kinetic realizations* of these consumer-resource systems admit a natural parameterization in terms of the system's *elementary flux modes* (EFM). EFMs represent fundamental sub-circuits (sub-communities) within the full circuit whose activity levels form a *flux parameterization* of the system. This allows one to write the linearization of the system about its equilibria as an *affine parameter dependent* (APD) system whose robust stability margin provides a direct characterization of the system's D2B with respect to its flux parameters. Since robust stability for APD systems can be cast in terms of linear matrix inequalities, this approach provides a computationally tractable method for assessing a system's D2B.

The following sections review background material on bifurcations of nonlinear dynamical systems. The chapter shows how to construct kinetic realizations and flux parameterizations of consumer-resource systems. The

D2B problem is then formulated as a robust stability problem for an APD system. The methodology is demonstrated using the tritrophic food web shown in Fig. 9.

1. Distance to Local Bifurcations (D2B)

This section reviews background material on system bifurcations and then defines the distance to local bifurcation or D2B of a system equilibrium. Let us consider a dynamical system whose orbit $x(\cdot; p) : \mathbb{R} \to \mathbb{R}^n$ satisfies

$$\dot{x}(t) = f(x(t); k_0) \tag{7}$$

with $x(0; p) = p$ and where $f : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n$ is locally Lipschitz in x and $k_0 \in \mathbb{R}^m$ is a *constant* vector of *nominal parameters*.

Now consider a perturbation of the nominal system whose orbits $z(\cdot; p) : \mathbb{R} \to \mathbb{R}^n$ satisfy

$$\dot{z}(t) = f(z(t), k_0 + \delta k) \tag{8}$$

with $z(0; p) = p$ and where $\delta k \in \mathbb{R}^m$ is a vector of parameter perturbations. We say a map $h : \mathbb{R}^n \to \mathbb{R}^n$ is a *homeomorphism* if h is continuous and h^{-1} exists and is continuous. The nominal system in equation (7) is *structurally stable* if and only if there exists $\epsilon > 0$ such that for any parameter perturbation with $|\delta k| < \epsilon$ there exists a homeomorphism h that maps orbits, x, of the nominal system onto the orbits, z, of the perturbed system while preserving the direction of time. If the nominal system is not structurally stable, then we say the system undergoes a *bifurcation* at parameter k_0.

Consider the dynamical system

$$\dot{x}(t) = f(x(t); k(t)) \tag{9}$$

where $f : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n$ is locally Lipschitz in x. We say the system undergoes a *bifurcation-induced regime shift* at time t_0 if the constant parameter system

$$\dot{z}(t) = f(z(t), k(t_0)) \tag{10}$$

is not structurally stable. If the above constant parameter system in equation (10) is structurally stable, then we define its distance-to-bifurcation as

$$\text{D2B} = \inf_{\delta k \in \mathbb{R}^m} \{|\delta k| \, : \, \dot{z} = f(z, k(t_0) + \delta k) \text{ is not structurally stable}\}$$

Finding the D2B can be computationally intractable unless all bifurcations are *local*. Consider the nominal system in equation (7) and let x^* be an equilibrium point such that $f(x^*; k_0) = 0$. We say this system is *locally topologically equivalent* at x^* to the perturbed system in equation (8) if there exists a neighborhood U of equilibrium x^* and there exists a function $h : \mathbb{R}^n \to \mathbb{R}^n$ such that

- there is a neighborhood V of a fixed point z^* of the perturbed system (i.e. $0 = f(z^*, k_0 + \delta k)$) over which h is a homeomorphism between U and V with $z^* = h(x^*)$ and $V = h(U)$.
- any of the nominal system orbits in U are mapped through h onto a perturbed system orbit in V while preserving the direction of time.

We say the nominal system is *locally structurally stable* at equilibrium x^* if and only if there exists $\epsilon > 0$ such that for any parameter perturbation with $|\delta k| < \epsilon$, we know the nominal and perturbed systems are locally topologically equivalent at x^*. If the nominal system is not locally structurally stable at x^*, then we say it undergoes a *local bifurcation* at parameter k_0. We may then define a *local* bifurcation-induced regime shift and its *local* D2B in the same way as was done for global bifurcations. The remainder of the monograph focuses on local D2B, so the "local" qualifier will be dropped if the type of bifurcation (global or local) is clear from the discussion's context.

Let x^* be an equilibrium of the nominal system $\dot{x} = f(x; k_0)$. The linearization of that system about x^* is the linear system

$$\dot{x}(t) = \mathbf{A}x(t)$$

where $\mathbf{A} = \left[\frac{\partial f(x;k_0)}{\partial x}\right]_{x=x^*}$ is a real-valued constant matrix called the linearization's system matrix. For a given system matrix, $\mathbf{A}$, we let n^+ denote the number of eigenvalues for system matrix $\mathbf{A}$ with positive real parts, n^0 denotes the number of eigenvalues with zero real parts, and n^- denotes the number of eigenvalues with negative real parts. We will call the triple, (n^+, n^0, n^-) the *stabiliy index* of the linearization at x^*. We say the equilibrium, x^*, is *hyperbolic* if $n^0 = 0$ (i.e. $\mathbf{A}$ has no eigenvalues with zero real parts).

The Hartmann-Grossman theorem [49] can be used to prove that the nominal system and its perturbation are locally topologically equivalent at a *hyperbolic* equilibrium, x^*, if and only if the linearizations of both systems have the same stability indices. So let $\mathbf{A}$ be the system matrix for a hyperbolic equilibrium, then there exists a similarity transformation $\mathbf{T}$ such that $\begin{bmatrix} \mathbf{A}_s & 0 \\ 0 & \mathbf{A}_u \end{bmatrix} = \mathbf{T}\mathbf{A}\mathbf{T}^{-1}$ where all of the eigenvalues of $\mathbf{A}_s$ and $-\mathbf{A}_u$ have negative real parts. Assessing the D2B at x^* is therefore equivalent to assessing the robust stability of a linear system with system matrix

$$\overline{\mathbf{A}} = \mathbf{T}^{-1} \begin{bmatrix} \mathbf{A}_s & 0 \\ 0 & -\mathbf{A}_u \end{bmatrix} \mathbf{T}$$

This reduces the problem of finding the distance to local bifurcation to a linear robust stability problem.

Remark: There are local structurally stable systems that are not (globally) structurally stable [71]. Necessary and sufficient conditions for global bifurcations exist for planar systems and for a restricted class of gradient-like

systems [103, 82]. These conditions, however, are difficult to verify computationally which is why this monograph confines itself to regime shifts triggered by local bifurcations.

Posing the problem of finding an equilibrium's D2B in terms of robust stability, however, is still complicated by the fact that parameter perturbations also perturb the system's equilibrium point. This means that the eigenvalues of the linearization depend in a complex manner on system parameters and this complexity can make it difficult to solve the linearization's robust stability problem. Our approach to this issue takes advantage of the fact that compartmental polynomial systems have realizations that are affine functions of the *fluxes* between compartments. These realizations are sometimes called *kinetic realizations* and the parameters characterizing their inter-compartmental fluxes are called *normalized flux parameters*. The following sections, 2 and 3, discuss flux parameterizations of kinetic realizations. Section 4 uses these parameterized realizations to solve the D2B problem for consumer-resource systems.

2. Kinetic Realizations of Consumer-Resource Systems

The compartmental dynamical system , $\dot{x} = f(x;k)$, has a *kinetic realization* if $f(x;k)$ can be written as an affine function of the fluxes between system compartments. This section discusses kinetic realizations of consumer-resource systems.

In the following it will be convenient to introduce the following notational conventions. A polynomial, $f(x;k)$ with indeterminate variables $x = \{x_1, \ldots, x_n\}$ and non-negative parameters $k = \{k_1, \ldots, k_m\}$ is a formal series

$$f(x;k) = \sum_{j=1}^{m} \left\{ \pm k_j \prod_{\ell=1}^{n} x_\ell^{y_{j\ell}} \right\} \tag{11}$$

where $y_{j\ell}$ are non-negative integers for $j = 1, 2, \ldots, m$ and $\ell = 1, 2, \ldots, n$. The set of all such polynomials whose parameters k take values in the real field is denoted as $\mathbb{R}[x]$ or $\mathbb{R}[x_1, \ldots, x_n]$. If the parameter k is treated as a variable, then the set of polynomials is denoted as $\mathbb{R}(k)[x]$. The set $\mathbb{R}[x]$ is an algebraic ring with respect to polynomial addition and multiplication. The n-dimensional row vector

$$\overline{y}_j = \begin{bmatrix} y_{j1} & y_{j2} & \cdots & y_{jn} \end{bmatrix}$$

for $= 1, 2, \ldots, n$ is called a *multi-index* and we denote the monomial generated by multi-index $\overline{y}$ as $x^{[\overline{y}]}$. Let $\mathbf{Y} \in \mathbb{Z}^{m \times n}$ be an integer matrix whose rows are the multi-indices of the monomial terms in the formal series, $f(x; k)$, of equation (11). We denote the m-vector of monomials in the formal series $f(x; k)$ as

$$x^{[\mathbf{Y}]} = \begin{bmatrix} k_1 x^{[\overline{y}_1]} & k_2 x^{[\overline{y}_2]} & \cdots & k_3 x^{[\overline{y}_m]} \end{bmatrix}^T$$

Now consider a dynamical system whose state trajectory $x : \mathbb{R} \to \mathbb{R}^n$ satisfies $\dot{x}(t) = f(x(t); k)$ where f is a vector of n polynomials in $\mathbb{R}(k)[x]$ with n variables $\{x_1, \ldots, x_n\}$ and m real parameters $k = \{k_1, \ldots, k_m\}$. This system is said to have a *kinetic realization*, $(\mathbf{N}, \mathbf{Y}, \mathbf{D}_k)$, if the system equations can be written as

$$\dot{x}(t) = \mathbf{N}\mathbf{D}_k x^{[\mathbf{Y}]}$$

where for some integer $p \geq m$ the matrix, $\mathbf{Y}$, is a $p \times n$ matrix whose rows are multi-indices, $\mathbf{N}$ is an $n \times p$ incidence matrix for a directed graph $G = (V, E)$ whose vertex set, V, consists of the multi-indices in $\mathbf{Y}$, and $\mathbf{D}_k$ is a $p \times p$ diagonal matrix whose diagonal elements are drawn from the system parameters $k = \{k_1, \ldots, k_m\}$.

Kinetic realizations often appear in chemical reaction networks with mass action kinetics. A sufficient condition for a non-negative polynomial system, $\dot{x} = f(x; k)$, to have a kinetic realization is that for all $i = 1, 2, \ldots, n$,

there exist polynomials $g_i(x;k)$ and $h_i(x;k)$ in $\mathbb{R}(k)[x]$ such that

$$f_i(x;k) = g_i(x;k) - x_i h_i(x;k)$$

A constructive proof for this condition was presented in [48].

Even though consumer-resource systems are not polynomial, one can still construct a kinetic realization through time scaling. Let us do this for the following tritrophic food web

$$\begin{aligned} \dot{x}_1 &= r_1 x_1 \left(1 - \tfrac{1}{K} x_1\right) - r_1 \tfrac{x_1 x_2}{1+x_1} \\ \dot{x}_2 &= r_2 \tfrac{x_1 x_2}{1+x_1} - r_3 \tfrac{x_2 x_3}{1+x_2} - m_1 x_2 \\ \dot{x}_3 &= r_3 \tfrac{x_2 x_3}{1+x_2} - m_3 x_3 \end{aligned}$$

where x_1 denotes the producer biomass, x_2 is the primary consumer's biomass and x_3 is the secondary consumer's biomass. The system parameters are K (carrying capacity), r_i (ith guild's growth rate), and m_i (ith guilds death rate). If we introduce the following time transformation

$$\tau(1 + x_1)(1 + x_2) = t$$

then we get the state equations

$$\begin{aligned} \dot{x}_1 &= r_1 x_1 \left(1 - \tfrac{1}{K} x_1\right)(1 + x_1)(1 + x_2) - r_2(1 + x_2) \\ \dot{x}_2 &= r_2 x_1 x_2 (1 + x_2) - r_3 x_2 x_3 (1 + x_2) \\ &\quad - m_1 x_2 (1 + x_1)(1 + x_2) \\ \dot{x}_3 &= r_3 x_2 x_3 (1 + x_1) - m_3 x_3 (1 + x_1)(1 + x_2) \end{aligned} \tag{12}$$

which is a polynomial realization for the original system equations.

Let us fix the value of some system parameters

$$r_1 = \frac{1}{2}, \quad , r_2 = \frac{5}{3}, \quad r_3 = \frac{1}{20}$$

and introduce perturbations on the producer's carrying capacity and the secondary consumer's mortality rate,

$$\frac{1}{K} = \frac{3}{2} + k_1, \quad m_2 = \frac{2}{5}, \quad m_3 = \frac{1}{100} + k_2$$

The parameter, k_1, is generated by interventions taken by a resource manager to improve the carrying capacity of the lake. The parameter, k_2, is generated by policies used by a resource manager to encourage or restrict harvesting of the secondary consumer.

The right hand side of equation (12) consists of polynomials in the ring $\mathbb{R}(k)[x]$ where $x = \{x_1, x_2, x_3\}$ and $k = \{k_1, k_2\}$. We now construct a kinetic realization of the polynomial system in equation (12) following the methods outlined in [**48**]. In particular, we first form the multi-index matrix, $\mathbf{Y}$, for the distinct monomials terms in each equation. For the first equation in (12), we select these monomials and their coefficients to be

j	1	2	3	4	5	6	7
$\overline{y}_j$	$[3,1,0]$	$[3,0,0]$	$[2,1,0]$	$[2,0,0]$	$[1,2,0]$	$[1,1,0]$	$[1,0,0]$
$x^{[\overline{y}_j]}$	$x_1^3x_2$	x_1^3	$x_1^2x_2$	x_1^2	$x_1x_2^2$	x_1x_2	x_1
$\mathbf{D}_k(j,j)$	$-\frac{9}{4}-\frac{3k_1}{2}$	$-\frac{9}{4}-\frac{3k_1}{2}$	$-\frac{3}{4}-\frac{3k_1}{2}$	$-\frac{3}{4}-\frac{3k_1}{2}$	$-\frac{5}{3}$	$-\frac{1}{6}$	$-\frac{3}{2}$

In practice, the computation of the above table would be implemented using a computer algebra tool such as `SINGULAR`, `Mathematica`, or `Maple`. Repeating the steps used to compute the above table for the other equations in (12) creates the kinetic realization for this system that is shown in Fig. 12. This realization will be used in later sections to demonstrate how one solves for the D2B.

3. Normalized Flux Parameters of Kinetic Systems

Kinetic realizations express the system equations as an affine function of the inter-compartmental fluxes. In particular, note that kinetic realization, $(\mathbf{N}, \mathbf{Y}, \mathbf{D}_k)$, allows one to rewrite the system equations as

$$\dot{x}(t) = f(x;k) = \mathbf{N}v(x;k)$$

where

$$v(x;k) = \mathbf{D}_k x^{[\mathbf{Y}]}$$

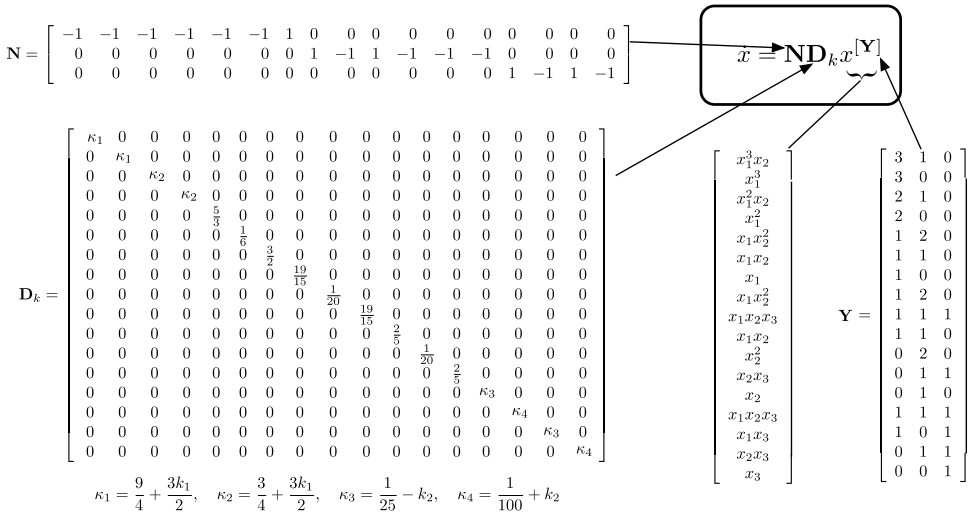

FIGURE 12. Kinetic Realization of Tritrophic Food Web

We refer to the p-dimensional vector $v(x;k)$ as the realization's *flux vector*. Since $\mathbf{N}$ is the incidence matrix of a graph with vertex set given by the monomials in $x^{[\mathbf{Y}]}$, one may view $v(x;k)$ as a flux between the vertices of this graph.

Let $x^*(k)$ denote an equilibrium for a kinetic realization $(\mathbf{N}, \mathbf{Y}, \mathbf{D}_k)$. Define the *flux equilibrium*

$$v^*(k) := v(x^*;k) = \mathbf{D}_k \left(x^*(k)\right)^{[\mathbf{Y}]}$$

Since $f(x^*(k);k) = 0$, one can readily deduce that the flux equilibrium, $v^*(k)$, is a non-negative vector in the null space of the kinetic system's incidence matrix, $\mathbf{N}$. In other words,

$$v^*(k) \in K_v := \ker(\mathbf{N}) \cap \mathbb{R}^p_{\geq 0}$$

K_v is called the realization's *equilibrium flux cone*. Note that the flux cone is a closed convex polyhedral set formed from the intersection of $\mathbf{N}$'s null space with the non-negative orthant in the parameter space, $\mathbf{R}^p_{\geq 0}$.

Since the flux cone, K_v, is a convex polyhedral set, it is finitely generated by a set of r *elementary flux modes* (EFM), $\{\overline{e}_1, \ldots, \overline{e}_r\}$. This set consists of non-negative vectors in the flux space that are *extreme rays* from which K_v is generated. This set of EFMs is unique and they are elementary in the sense that no EFM can be written as a positive linear combination of other EFMs. This means that any equilibrium flux v^* in the flux cone, K_v, can be written as $v^* = \mathbf{E}\lambda$ where $\mathbf{E}$ is a $p \times r$ matrix whose ith column is the EFM, $\overline{e}_i$, and $\lambda = [\lambda_1, \ldots, \lambda_r]$ is an r-vector of flux parameters. So an alternative representation of the flux cone is

$$K_v = \left\{ v \in \mathbb{R}^p_{\geq 0} \,:\, v \in \mathbf{E}\lambda, \quad \lambda \in \mathbb{R}^r_{\geq 0} \right\}$$

Remark: The EFM matrix, $\mathbf{E}$, of a kinetic realization $(\mathbf{N}, \mathbf{Y}, \mathbf{D}_k)$ is efficiently computed [**38, 66, 115**] from binary encodings of the realization's incidence matrix $\mathbf{N}$.

Let us assume we've found the EFM matrix, $\mathbf{E}$ for a kinetic realization of the system, $\dot{x} = f(x;k)$, with real parameter $k \in \mathbb{R}^q_{\geq 0}$ and let x^* be an equilibrium for this system. As mentioned above, the equilibrium flux, $v^* = v(x^*;k)$, associated with this equilibrium can be written as $v^* = \mathbf{E}\lambda$. The linearization's system matrix can be shown to be

$$\mathbf{A} = \left[\frac{\partial f(x;k)}{\partial x} \right]_{x=x^*} = \mathbf{N}\mathrm{diag}(\mathbf{E}\lambda)\mathbf{Y}\mathrm{diag}(h) \tag{13}$$

where $h = 1/x^*$ is a vector whose components are reciprocals of the components in x^*. Note that the system matrix in equation (13) is dependent on the components in λ and h. But if one were to multiply out equation (13), we would see that $\mathbf{A}$ is *affine* with respect to monomials of the form $\lambda_i h_j$. This suggests that it would be better to define a set of *normalized flux parameters*

$$\mu = \{\mu_1, \ldots, \mu_q\}$$

where each μ_ℓ represents a product of a flux parameter λ_i and the reciprocal of a component of the equilibrium, h_j. So the system matrix $\mathbf{A}$ is now affine in the sense that there exist matrices $\{\mathbf{A}_\ell\}_{\ell=1}^{q}$ such that

$$\mathbf{A} = \sum_{\ell=1}^{q} \mu_\ell \mathbf{A}_\ell \tag{14}$$

We refer to μ as the *normalized flux parameters* associated with the kinetic realization and in bounding the system's distance-to-local bifurcation we will do this with respect to perturbations of the normalized flux parameters, μ.

Let us now determine the affine parameterization for the tritrophic food web whose kinetic realization was shown in Fig. 12. The EFM matrix for this system was computed using `efmtool` [**115**]. The resulting matrix is shown in Fig. 13(a). The relationships between the equilibrium fluxes v^* and $\mathbf{E}\lambda$ are shown in Fig. 13(b). Computer algebra tools were used to form the Jacobian matrix according to equation (13). This yielded a 3×3 matrix (Fig. 13(c)) whose elements are affine functions of the normalized flux parameters shown in Fig. 13(d).

4. Distance to Local Bifurcation of Kinetic Systems

With the affine parameterization of the linearization's system matrix as shown in equation (14) one can now compute a bound on the D2B for a specified equilibrium, x^*. This section first computes that bound when x^* is an *asymptotically stable* and *positive* equilibrium. The end of the section discusses how one can relax this to any non-negative hyperbolic equilibrium.

Let us introduce the following notational conventions,

$$\mathbf{I}_h = \mathrm{diag}(h), \quad \tilde{\mathbf{J}}(\lambda) = \mathbf{N}\mathrm{diag}(\mathbf{E}\lambda)\mathbf{Y}$$

(a) EFM matrix for food web

$$\mathbf{E} = \begin{bmatrix} 001000000000000000 \\ 000100000000000000 \\ 000010000000000000 \\ 000001000000000000 \\ 100000000000000000 \\ 010000000000000000 \\ 111111000000000000 \\ 000000101001100000 \\ 000000001100000000 \\ 000000010110010000 \\ 000000100000010000 \\ 000000010000100000 \\ 000000000011000000 \\ 000000000000001010 \\ 000000000000001100 \\ 000000000000000101 \\ 000000000000000011 \end{bmatrix}$$

(b) EFM parameterization of equilibrium fluxes

$$\begin{array}{lcll} v_1^* & = & \left(\frac{9}{4}+\frac{3k_1}{2}\right)x_1^3x_2 & = \lambda_3 \\ v_2^* & = & \left(\frac{9}{4}+\frac{3k_1}{2}\right)x_1^3 & = \lambda_4 \\ v_3^* & = & \left(\frac{3}{4}+\frac{3k_1}{2}\right)x_1^2x_2 & = \lambda_5 \\ v_4^* & = & \left(\frac{3}{4}+\frac{3k_1}{2}\right)x_1^2 & = \lambda_6 \\ v_5^* & = & \frac{5}{3}x_1x_2^2 & = \lambda_1 \\ v_6^* & = & \frac{1}{6}x_1x_2 & = \lambda_2 \\ v_7^* & = & \frac{3}{2}x_1 & = \lambda_1+\lambda_2+\lambda_3+\lambda_4+\lambda_5+\lambda_6 \\ v_8^* & = & \frac{19}{15}x_1x_2^2 & = \lambda_7+\lambda_9+\lambda_{12}+\lambda_{13} \\ v_9^* & = & \frac{1}{20}x_1x_2x_3 & = \lambda_9+\lambda_{10} \\ v_{10}^* & = & \frac{19}{15}x_1x_2 & = \lambda_8+\lambda_{10}+\lambda_{11}+\lambda_{14} \\ v_{11}^* & = & \frac{2}{5}x_2^2 & = \lambda_7+\lambda_{14} \\ v_{12}^* & = & \frac{1}{20}x_2x_3 & = \lambda_8+\lambda_{13} \\ v_{13}^* & = & \frac{2}{5}x_2 & = \lambda_{11}+\lambda_{12} \\ v_{14}^* & = & \left(\frac{1}{25}-k_2\right)x_1x_2x_3 & = \lambda_{15}+\lambda_{17} \\ v_{15}^* & = & \left(\frac{1}{100}+k_2\right)x_1x_3 & = \lambda_{15}+\lambda_{16} \\ v_{16}^* & = & \left(\frac{1}{25}-k_2\right)x_2x_3 & = \lambda_{16}+\lambda_{18} \\ v_{17}^* & = & \left(\frac{1}{100}+k_2\right)x_3 & = \lambda_{17}+\lambda_{18} \end{array}$$

(c) Affine Parameterization of System Matrix in terms of normalized flux parmaters, μ

$$\mathbf{A}(\mu) = \begin{bmatrix} -2\mu_2-2\mu_4-\mu_6-\mu_7 & -2\mu_1-\mu_3-\mu_5-\mu_8 & 0 \\ \mu_9+\mu_{10}+\mu_{13}+\mu_{15}+\mu_{17}+\mu_{19} & \mu_{11}+\mu_{18}+\mu_{20}-\mu_{21} & -\mu_{12}-\mu_{14}-\mu_{16}-\mu_{22} \\ \mu_{25}-\mu_{23} & \mu_{24}+\mu_{26}+\mu_{27}+\mu_{28} & 0 \end{bmatrix}$$

(d) Normalized Flux Mode Parameters

$$\begin{array}{ccccccc} \mu_1=h_2\lambda_1 & \mu_2=h_1\lambda_3 & \mu_3=h_2\lambda_2 & \mu_4=h_1\lambda_4 & \mu_5=h_2\lambda_3 & \mu_6=h_1\lambda_5 & \mu_7=h_1\lambda_6 \\ \mu_8=h_2\lambda_5 & \mu_9=h_1\lambda_7 & \mu_{10}=h_1\lambda_8 & \mu_{11}=h_2\lambda_9 & \mu_{12}=h_3\lambda_8 & \mu_{13}=h_1\lambda_{11} & \mu_{14}=h_3\lambda_9 \\ \mu_{15}=h_1\lambda_{12} & \mu_{16}=h_3\lambda_{10} & \mu_{17}=h_1\lambda_{13} & \mu_{18}=h_2\lambda_{12} & \mu_{19}=h_1\lambda_{14} & \mu_{20}=h_2\lambda_{13} & \mu_{21}=h_2\lambda_{14} \\ \mu_{22}=h_3\lambda_{13} & \mu_{23}=h_1\lambda_{16} & \mu_{24}=h_2\lambda_{15} & \mu_{25}=h_1\lambda_{17} & \mu_{26}=h_2\lambda_{16} & \mu_{27}=h_2\lambda_{17} & \mu_{28}=h_2\lambda_{18} \end{array}$$

FIGURE 13. EFM matrix, parameterization of equilibrium fluxes, affine parameterization of system matrix

Since we assumed the equilibrium was positive, all entries of $\mathbf{I}_h$ are well defined. The linearization's system matrix may therefore be written as

$$\mathbf{A} = \tilde{\mathbf{J}}(\lambda)\mathbf{I}_h$$

With these conventions, the linearized state equations become

$$\frac{d}{dt}(x - x^*) = \tilde{\mathbf{J}}(\lambda)\mathbf{I}_h(x - x^*)$$

We then introduce the following change of variables

$$z = \mathbf{I}_h(x - x^*)$$

Since $\dot{z} = \mathbf{I}_h \dot{x}$, we can readily see that the linearized system equation becomes

$$\dot{z} = \mathbf{I}_h \tilde{\mathbf{J}}(\lambda) = \mathbf{A}(\mu) z$$

where we explicitly note the system matrix' dependence on the normalized flux parameters, μ. Because we assumed the equilibrium, x^*, was asymptotically stable and positive, the matrix $\mathbf{A}(\mu)$ is well defined and the origin of this system is asymptotically stable.

Now let k_0 be a *nominal parameter* for the original system and let $x^*(k_0)$ denote an equilibrium associated with that nominal parameter. There must be a vector $\lambda_0 \in \mathbb{R}^r_{\geq 0}$ such that the equilibrium flux at this nominal equilibrium satisfies

$$v(x^*(k_0); k_0) = \mathbf{E}\lambda_0$$

where $\mathbf{E}$ is the system's EFM matrix. Since all components of x^* are positive, this means there is a "nominal" normalized flux vector μ_0 such that the normalized flux parameters can be written as

$$\mu = \mu_0 + \tilde{\mu}$$

In other words, the affine parameterization of the system matrix in equation (14) can be written as

$$\begin{aligned} \mathbf{A}(\mu) &= \sum_{i=1}^{q} \mu_i \mathbf{A}_i = \sum_{i=1}^{q} (\mu_{0i} + \tilde{\mu}_i)\mathbf{A}_i \\ &= \mathbf{A}_0 + \sum_{i=1}^{q} \tilde{\mu}_i \mathbf{A}_i \end{aligned} \tag{15}$$

where $\tilde{\mu}$ denotes a perturbation about the nominal normalized flux parameter, μ_0 and $\mathbf{A}_0 = \sum_{i=1}^{q} \mu_{0i}\mathbf{A}_i$. Note that while there are q matrices in the sum, many of these matrices are duplicates. So it will be more convenient

to rewrite equation (15) as

$$\mathbf{A} = \mathbf{A}_0 + \sum_{i=1}^{\tilde{q}} \rho_i(\tilde{\mu})\tilde{\mathbf{A}}_i \tag{16}$$

where $\tilde{q} \leq q$ is an integer such that $\{\tilde{\mathbf{A}}_i\}_{i=1}^{\tilde{q}}$ is the set of *distinct* matrices in equation (15)'s sum and $\rho_i(\tilde{\mu})$ is a linear function of the perturbations about the nominal normalized flux parameter, μ_0.

If we treat $\{\rho_i(\tilde{\mu})\}_{i=1}^{\tilde{q}}$ as a parameter, then equation (16) is the uncertain system matrix for an *affine parameter dependent system* (APD) of the form

$$\dot{z} = \left(\mathbf{A}_0 + \sum_{i=1}^{\tilde{q}} \rho_i \tilde{\mathbf{A}}_i\right) z \tag{17}$$

that was studied in [39]. That paper established sufficient conditions for the robust stability of the uncertain linear system in equation (17). In particular, let $\Gamma \subset \mathbb{R}^{\tilde{q}}$ be a convex polytope containing the origin and that is generated by the following set $\{\gamma_\ell\}_{\ell=1}^{N}$ of points in the parameter space. From [39], a sufficient condition for the system matrix

$$\mathbf{A}(\rho) := \mathbf{A}_0 + \sum_{i=1}^{\tilde{q}} \rho_i \tilde{\mathbf{A}}_i \tag{18}$$

to be Hurwitz for any $\rho = \{\rho_1, \ldots, p_{\tilde{q}}\}$ in Γ is that $\mathbf{A}_0$ is Hurwitz and that there exist $\tilde{q}+1$ symmetric matrices $\mathbf{Q}_0, \mathbf{Q}_1, \ldots, \mathbf{Q}_{\tilde{q}}$ such that the parameter dependent matrix

$$\mathbf{Q}(\rho) = \mathbf{Q}_0 + \rho_1\mathbf{Q}_1 + \cdots + \rho_{\tilde{q}}\mathbf{Q}_{\tilde{q}} \tag{19}$$

satisfies

$$\mathbf{A}^T(\gamma_i)\mathbf{Q}(\gamma_i) + \mathbf{Q}(\gamma_i)\mathbf{A}(\gamma_i) < 0 \tag{20}$$

for $i = 1, 2, \ldots, N$ with

$$\tilde{\mathbf{A}}_i^T\mathbf{Q}_i + \mathbf{Q}_i\tilde{\mathbf{A}}_i \geq 0 \tag{21}$$

for $i = 0, 1, 2, \ldots, \tilde{q}$.

These conditions establish that

$$V(x;\rho) = x^T \mathbf{Q}(\rho) x$$

is a parameter dependent Lyapunov function [4] for any system $\dot{z} = \mathbf{A}(\rho)z$ with $\rho \in \Gamma$. In particular equations (20-21) are linear matrix inequalities (LMI) with matrix variables $\mathbf{Q}_0, \mathbf{Q}_1, \ldots, \mathbf{Q}_{\tilde{q}}$. Since LMI problems are a class of convex optimization problem for which efficient interior point algorithms exist, it means that certifying the robust stability of the system $\dot{x} = \mathbf{A}(\rho)z$ is computationally tractable using tools such `pdlstab` in MATLAB's robust control toolbox [40].

Let us now see how this works for the positive stable equilibria of the tritrophic food web. The kinetic realization, $(\mathbf{N}, \mathbf{D}_k, \mathbf{Y})$, is shown in Fig. 12 and the EFM matrix and normalized flux parameters are shown in Fig. 13. To certify the robust stability of the nominal system, we first find all of the system equilibria by solving the following set of polynomial equations,

$$\begin{aligned} 0 &= r_1 x_1 \left(1 - \tfrac{x_1}{K}\right)(1 + x_1) - r_2 x_1 x_2 \\ 0 &= r_2 x_1 x_2 (1 + x_2) \\ &\quad -r_3 x_2 x_3 (1 + x_1) - m_2 x_2 (1 + x_1)(1 + x_2) \\ 0 &= r_3 x_2 x_3 - m_3 x_3 (1 + x_2) \end{aligned} \tag{22}$$

using the nominal parameter values given before. All solutions to these polynomial equations may be computed using triangular decompositions of the Groebner basis for the ideal formed from these polynomials [22]. We computed these equilibria using functions in the computer algebra tool SINGULAR [42]. The resulting equilibria are shown below in Table 1. Note that all of the equilibria are hyperbolic, so we know this system is locally structurally stable. Only one of the equilibria, however, is positive and stable. We construct an APD linearization at this positive/stable equilibrium and use the results from [39] to certify its robust stability. The end of the

section outlines how one could use this robust stability analysis for linearizations about the non-positive and/or unstable equilibria.

equilibrium x^*	Jacobian $\mathbf{A}$	eigenvalues	stability index (n^+, n^0, n^-)
$\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 1.5 & 0 & 0 \\ 0 & -0.4 & 0 \\ 0 & 0 & -0.01 \end{bmatrix}$	$\lambda_1 = 1.5$ $\lambda_2 = -0.4$ $\lambda_3 = -0.01$	$(1, 0, 2)$
$\begin{bmatrix} 0.67 \\ 0 \\ 0 \end{bmatrix}$	$\begin{bmatrix} -2.5 & -1.1 & 0 \\ 0 & 0.44 & 0 \\ 0 & 0 & -0.016 \end{bmatrix}$	$\lambda_1 = 0.44$ $\lambda_2 = -2.5$ $\lambda_3 = -0.016$	$(1, 0, 2)$
$\begin{bmatrix} 0.32 \\ 0.62 \\ 0 \end{bmatrix}$	$\begin{bmatrix} -1.11 & -0.85 & 0 \\ 1.28 & 0 & -0.04 \\ 0.00 & 0.00 & 0.02 \end{bmatrix}$	$\lambda_1 = 0.02$ $\lambda_2 = -0.55 + j.88$ $\lambda_3 = -0.55 - j.88$	$(1, 0, 2)$
$\begin{bmatrix} 0.54 \\ 0.25 \\ 4.73 \end{bmatrix}$	$\begin{bmatrix} -2.19 & -1.14 & 0 \\ 0.34 & 0.07 & -0.02 \\ 0 & 0.29 & 0 \end{bmatrix}$	$\lambda_1 = -.05 + j.05$ $\lambda_2 = -.05 - j.05$ $\lambda_3 = -2.01$	$(0, 0, 3)$

TABLE 1. Linearization of Tritrophic Food web

From Fig. 13 we saw there were 28 normalized flux parameters $\{\mu_i\}_{i=1}^{28}$. But when we look at the set of matrices $\{\mathbf{A}_i\}_{i=1}^{28}$, there are only 7 distinct matrices forming $\{\tilde{\mathbf{A}}_i\}_{i=1}^{7}$ as shown in Fig. 14. So the APD realization of our system is

$$\mathbf{A}(\tilde{\mu}) = \mathbf{A}_0 + \sum_{i=1}^{7} \rho_i(\tilde{\mu})\tilde{\mathbf{A}}_i$$

where the ρ_i are also shown in Fig. 14.

We then formulate a polytopic set Γ of uncertainties. In particular, we choose a box centered at the origin so that

$$\rho(\tilde{\mu}) \in [-R, R]^7 = \Gamma_R$$

where R is a scalar parameter representing the size of the uncertainty set, Γ_R. Once this is done, we use the function `pdlstab` in MATLAB's robust control tool box to verify the robust stability of $\mathbf{A}(\tilde{\mu})$ with respect to the

k	$\rho_k(\tilde{\mu})$	$\tilde{\mathbf{A}}_k$	k	$\rho_k(\tilde{\mu})$	$\tilde{\mathbf{A}}_k$
0	1	$\begin{bmatrix} -2.19 & -1.14 & 0 \\ 0.34 & 0.07 & -0.02 \\ 0 & 0.29 & 0 \end{bmatrix}$	4	$\tilde{\mu}_{13} - \tilde{\mu}_{11} + \tilde{\mu}_{15} + \tilde{\mu}_{17}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
1	$-2\tilde{\mu}_2 - 2\tilde{\mu}_4 - \tilde{\mu}_6 - \tilde{\mu}_7$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	5	$-\tilde{\mu}_{16} - \tilde{\mu}_{18} - \tilde{\mu}_{24} - \tilde{\mu}_{28}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}$
2	$-2\tilde{\mu}_1 - \tilde{\mu}_3 - \tilde{\mu}_5 - \tilde{\mu}_8$	$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	6	$\tilde{\mu}_{22} - \tilde{\mu}_{21}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$
3	$\tilde{\mu}_9 + \tilde{\mu}_{10} + \tilde{\mu}_{12} + \tilde{\mu}_{14}\tilde{\mu}_{19} + \tilde{\mu}_{26}$	$\begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	7	$\tilde{\mu}_{20} + \tilde{\mu}_{23} + \tilde{\mu}_{25} + \tilde{\mu}_{27}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$

FIGURE 14. Reduced APD Linearization of Tritrophic System

chosen uncertainty set. In particular, we embed this function in a bisection algorithm to find the largest R such that $\mathbf{A}(\tilde{\mu})$ has robust stability with respect to Γ_R. Applying this search to the tritrophic food web, we found the largest R for robust stability to be 0.0192. We can therefore take this as the distance to local bifurcation with respect to the parameter set $\{\rho_i(\tilde{\mu})\}_{i=1}^{7}$.

The distance computed above is overly conservative because it is determined by the maximum deviation with respect to all of the structured uncertainty matrices $\left\{\tilde{\mathbf{A}}_i\right\}_{i=1}^{7}$. The original problem statement only considered perturbations to the carrying capacity, K, and the secondary consumer's mortality rate, m_3. These two parameters strongly perturb only two of the structured uncertainty matrices; namely $\tilde{\mathbf{A}}_1$ and $\tilde{\mathbf{A}}_7$.

Let us first look at the D2B for perturbations, k_1, to $1/K$. If we look at the Fig. 14 we see that

$$\begin{aligned} \rho_1(\tilde{\mu}) &= -2\tilde{\mu}_2 - 2\tilde{\mu}_4 - \tilde{\mu}_6 - \tilde{\mu}_7 \\ &= -2\frac{\lambda_3}{x_1^*} - 2\frac{\lambda_4}{x_1^*} - \frac{\lambda_5}{x_1^*} - \frac{\lambda_6}{x_1^*} \\ &= 3k_1(x_1^*)^2(x_2^*) + 3k_1(x_1^*)^2 + 3k_1(x_1^*)(x_2^*) + 3k_1(x_1^*) \end{aligned}$$

Small perturbations in k_1 will generate small changes in the equilibrium x^*, so if we simply let x^* be the nominal equilibrium then the above equation

implies

$$|\tilde{\mu}_1| \;=\; 3.1728k_1$$

If we then use our preceding procedure to check the robust stability of the APD matrix

$$\mathbf{A}_0 + \tilde{\mu}_1\tilde{\mathbf{A}}_1$$

we get a bound of $D2B = 1$, which means $|k_1| < \frac{1}{3.1728} \approx 0.31$ to ensure robust stability to variations in the carrying capacity. This assertion can be readily verified through simulation where $1/K$ is perturbed away from its nominal value of $3/2$. Simulations show we can perturb $1/K$ by 0.53 before a local bifurcation is triggered. This result is consistent with the prediction made using the D2B analysis.

Now let us look at the D2B for perturbations, k_2, to the m_3. Again Fig. 14 implies

$$\begin{aligned}\rho_7(\tilde{\mu}) &= \tilde{\mu}_{24} + \tilde{\mu}_{26} + \tilde{\mu}_{27} + \tilde{\mu}_{28} \\ &= \frac{\lambda_{15}}{x_2^*} + \frac{\lambda_{16}}{x_2^*} + \frac{\lambda_{17}}{x_2^*} + \frac{\lambda_{18}}{x_2^*} \\ &= k_2\frac{x_1^*x_3^*}{x_2^*} + k_2\frac{x_3^*}{x_2^*}\end{aligned}$$

We again let x^* be the nominal equilibrum and evaluate the above equation to see that

$$|\tilde{\mu}_7| \;=\; 29.28k_2$$

Using our procedure to check the robust stability of the APD matrix

$$\mathbf{A}_0 + \tilde{\mu}_7\tilde{\mathbf{A}}_7$$

gives the bound $D2B = 0.29$ which means that $|k_2| < \frac{.29}{29} \approx .01$. This assertion is again checked through simulation where one sees that by reducing the secondary consumer's morality rate from 0.01 to 0.001 triggers a local bifurcation of the positive equilibrium. These results thereby suggest the

system is most sensitive to perturbations of the secondary consumer's mortality rate, rather than changes in producer carrying capacity. Results such as these, therefore, could be useful in advising an environmental resource manager to focus on regulating consumer harvesting (i.e. fishing) rather than using more expensive interventions that enhance the lake's carrying capacity.

Relaxing Restriction to Asymptotically Stable and Positive Equilibria: The prior example confined its attention to linearizations about asymptotically stable and positive equilibria of the kinetic realization. We need to relax this restriction to assess the D2B for the other non-positive and unstable hyperbolic equilibria of the realization.

The restriction to positive equilibria may be relaxed by noting that if a non-negative equilibrium has components that are identically zero, then those components will remain zero for all time. We can therefore remove those components from the system equations $\dot{x} = f(x;k)$ to obtain a lower dimensional system whose equilibria are all positive. One would then solve the D2B problem for this lower dimensional system.

The restriction to asymptotically stable equilibria can be relaxed by decomposing $\mathbf{A}(\tilde{\mu})$ with respect to its stable and unstable eigenvalues. In particular, the system matrix for the APD realization is

$$\mathbf{A}(\tilde{\mu}) = \mathbf{A}_0 + \sum_{i=1}^{\tilde{q}} \rho_i(\tilde{\mu})\tilde{\mathbf{A}}_i$$

and we know there exists a similarity transformation such that

$$\mathbf{T}\mathbf{A}_0\mathbf{T}^{-1} = \begin{bmatrix} \mathbf{A}_{0s} & 0 \\ 0 & \mathbf{A}_{0u} \end{bmatrix}$$

where $\mathbf{A}_{0s}$ and $\mathbf{A}_{0u}$ are Hurwitz. So consider

$$\begin{aligned}\mathbf{T}\mathbf{A}(\tilde{\mu})\mathbf{T}^{-1} &= \mathbf{T}\mathbf{A}_0\mathbf{T}^{-1} + \sum_{i=1}^{\tilde{q}} \rho_i(\tilde{\mu})\mathbf{T}\tilde{\mathbf{A}}_i\mathbf{T}^{-1} \\ &= \begin{bmatrix} \mathbf{A}_{0s} & 0 \\ 0 & \mathbf{A}_{0u} \end{bmatrix} + \sum_{i=1}^{\tilde{q}} \rho_i(\tilde{\mu})\mathbf{T}\tilde{\mathbf{A}}_i\mathbf{T}^{-1}\end{aligned}$$

Note that this is still an affine parameter dependent system but the first matrix in the sum is not Hurwitz. We address this issue by considering the robust stability of the modified affine parameter dependent matrix

$$\begin{bmatrix} \mathbf{A}_{0s} & 0 \\ 0 & \mathbf{A}_{0u} \end{bmatrix} + \sum_{i=1}^{\tilde{q}} \rho_i(\tilde{\mu})\mathbf{T}\tilde{\mathbf{A}}_i\mathbf{T}^{-1}$$

Since this is also an APD system, and since the first matrix in the sum is now Hurwitz, we can use our method to assess this modified system's robust stability, thereby providing a way to compute the D2B for hyperbolic equilibria that are not asymptotically stable.

5. Summary and Further Readings

Bifurcation-induced regime shifts occur when a perturbation of the system parameters causes a bifurcation of a structurally stable system. A sufficient condition for such a bifurcation is that the stability index of some equilibrium changes under the parameter perturbation. The smallest parameter perturbation triggering such a local bifurcation of the equilibrium is called the system's distance-to-bifurcation or D2B. This restriction to local bifurcations, allows us to treat the D2B problem as a robust stability problem for a linearization about the system's equilibria.

This chapter showed that kinetic realizations of consumer resource systems could be used to construct affine parameter dependent (APD) linearizations whose robust stability problem could be efficiently solved using existing tools for linear matrix inequalities (LMI). Parameter dependent robust stability problems were studied in [4], but the use of LMI's to solve the problem was pioneered in [39]. The LMI tool kit [40] used to solve this problem has been enormously influential in modern control theory.

Prior approaches to the D2B problem used numerical continuation [26, 25] to search for local bifurcations. More recent work has found the D2B by using the positivstellensatz theorem [105] to form semidefinite programs of sum-of-squares polynomials [110] or Handelmann polynomials [121]. All of these methods confine their attention to local bifurcations and they can only handle a limited number of parameters. Algorithmic methods have been used to search for global bifurcations [27] and heteroclinic orbits [28]. But this prior work is also greatly limited in the number of parameters it can treat. The APD method discussed in this chapter first appeared in [72] and was developed to address these scaling issues.

Kinetic realizations appear in the modeling of biochemical reaction networks. The characterization of the flux cone, K_v, will be found in [13]. The rays (elementary flux modes) generating the cone appear to form elementary circuits in biochemical networks [99] that play an important role in reducing the complexity of analyzing large biochemical networks [15]. The importance of these subnetworks has motivated the development of computational tools [115] capable of handling large networks. These tools play an important role in the study of cellular signal pathways.

The proposed solution to the D2B problem relied on recent advances in LMIs and convex optimization. But computing a system's kinetic realization, its flux parameterization, and finally identifying the structured uncertainty matrices in the APD system require extensive use of computer algebra systems [120]. Computer algebra plays a critical role in finding all system equilibria, in doing the tedious algebra for large-scale systems, and even providing computational "proofs" certifying a given system's properties. These computational tools will also be used in later chapters.