On the dynamical analysis of evolution equations via generalized models

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Abstract

The analysis of evolution equations such as ordinary or partial differential equations often splits into two different directions. One either makes minimal assumptions about their structure and tries to prove general theorems or one studies a particular model and analyzes its dynamics in detail. Generalized models provide a framework that allows to study evolution equation models without specifying all functional forms and they also provide enough flexibility to take into account insight from mathematical modeling. Although generalized models have been used successfully in many applications a structural mathematical approach that builds a bridge between theory and applications has not been developed yet. Here we provide this approach. We show the wide applicability of the method to ordinary, partial and functional differential equations. We also illustrate the dynamical analysis of generalized models via theoretical as well as practical examples.

Keywords: Generalized models, evolution equations, bifurcations, scaling transformation.

1 Introduction

Generalized models provide a method to analyze dynamical systems with unknown functional forms. We provide a structural overview on generalized models, their properties and their applications. The basic problem addressed by generalized models is that mathematical modeling can often not provide an exact set of evolution equations. This is particularly evident by comparing models from biophysics and classical physics as observed by Guckenheimer [23]:

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"The Hodgkin-Huxley models are based upon sound biophysical principles, but these principles do not constrain the models to a definite set of equations in the same manner that a few assumptions about fluid properties lead to the Navier-Stokes equations of fluid dynamics."

Therefore we always seem to face the dilemma that a dynamical analysis requires a given specified model. Once we specify some of the functions, that are only partially or not at all known, then we cannot provide a result that is valid for the underlying physical, chemical or biological process in full generality. Generalized models provide an intermediate alternative that allows the mathematical modeler to use much of the partial information he has available but still provides enough flexibility to treat many different alternative models simultaneously. Our goal here is to give a systematic treatment of generalized models and to detail all the basic results and ideas of the method. Furthermore, we show that the approach can be applied to a wide variety of evolution equations and is not limited to ordinary differential equations. We also develop several examples and highlight several applications to provide a comprehensive discussion. The main steps of the method are:

(G1) Build a model of the underlying process as evolution equations and group different terms in the resulting equations.

(G2) Apply a normalizing re-scaling transformation in phase space based on the existence of an equilibrium point and introduce so-called generalized parameters.

(G3) Interpret the generalized parameters in the modeling context.

(G4) Apply methods such as bifurcation analysis to characterize the dynamics of the generalized model.

We note that steps (G2) and (G4) are rigorous mathematical steps that provide one part of the method. The steps (G1) and (G3) are based on the application and the design of an appropriate mathematical model. Both parts have to be applied together for a generalized modeling approach to succeed. Several approaches exist that contain ideas similar to generalized modeling. For example, S-systems [46, 8] group different terms of the evolution equations. Metabolic control theory [36, 30, 44] considers the idea of a linearized analysis for a dynamical system using sensitivities; see also Section 3. The idea of re-scaling to simplify or de-singularize a problem appears in mathematical approaches for analyzing nonlinear systems; a typical example is provided by the blow-up method [5, 6] that can be viewed as a phase space re-scaling in suitable coordinates. However, it is important to point out that the combination of the different ideas in the framework of generalized models provides a very refined and flexible method.

In Section 2 we introduce generalized models for arbitrary ordinary differential equations in an arbitrary number of dimensions. We also carry out the normalizing transformation and prove some of its basic properties for completeness. In Section 3 the generalized parameters are introduced and their role in the stability and bifurcation analysis is indicated. This completes the formal construction of the generalized model. In Section 4 several examples are developed that provide details what information can or cannot be inferred from a bifurcation analysis of a generalized model. In Section 5 we demonstrate that generalized models can

also be applied to partial, delay and stochastic differential equations. This shows that the modeling approach covers a wide variety of evolution equations. In Section 6 we discuss three successful applications of generalized models. Each application highlights a different aspect of the possible conclusions and modeling approaches.

2 Generalized Models

We start by introducing generalized models for ordinary differential equations (ODEs). A general autonomous first-order system of ODEs is given by

$$\frac{dX}{dt} = X' = F(X;\mu) \tag{1}$$

where $X \in \mathbb{R}^n$ are phase space variables, $\mu \in \mathbb{R}^p$ are parameters and the vector field $F : \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^n$ is assumed to be at least continuously differentiable in X and continuous in μ. If we can specify a particular map F then the main task is to analyze the dynamics of (1) i.e. to partition the parameter space $\mathbb{R}^p$ into regions of qualitatively equivalent dynamics [41]. If we do not specify any assumptions on F we focus on the abstract analysis of ODEs [27]. Generalized models provide one possibility to bridge the gap between specific models and abstract analysis by making some structural assumptions on F without specifying the map completely. We assume that (1) has a `decomposition` of the form

$$X_i' = F_i(X;\mu) = \sum_{k=1}^{K_i} a_{i,k} F_{i,k}(X;\mu), \qquad \text{for } a_{i,k} \in \{-1, 1\}, \tag{2}$$

where the subscript $i \in \{1, 2, \ldots, n\}$ indicates the i-th coordinate, $K_i \geq 2$ and $F_i, F_{i,k} : \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^+$. We call terms $F_{i,k}$ with $a_{i,k} = 1$ `gain terms` and those with $a_{i,k} = -1$ `loss terms`. We note that the type of decomposition is decided as part of the mathematical modeling and does not follow a fixed set of rules. Therefore we can always decide how to choose $F_{i,k}$ and K_i; it should be noted that the basic principle of grouping the different terms is often provided by their role in the mathematical model. To illustrate the abstract theory of generalized models we are also going to use the simple model system given in the next example.

Example 2.1. Consider an ecological system [21] with prey X_1 and predators X_2 given by

$$\begin{aligned} X_1' &= F_{1,1}(X_1;\mu) - F_{1,2}(X_1, X_2;\mu) \\ X_2' &= F_{2,1}(X_1, X_2;\mu) - F_{2,2}(X_2;\mu) \end{aligned} \tag{3}$$

where $F_{1,1}(X_1;\mu)$ describes growth of the prey, $F_{2,2}(X_2;\mu)$ is natural mortality of the predator and we assume that $F_{1,2}(X_1, X_2;\mu) = F_{2,1}(X_1, X_2;\mu)$ is the predator-prey interaction i.e. X_1 is consumed by X_2. Note that the decomposition of the predator-prey model into gain and loss terms is basically prescribed by the mathematical modeling.

A first step to understand the dynamics of (1) is to analyze the stability and bifurcations of equilibria. Suppose there exists an equilibrium point X^* so that $F(X^*) = 0$. The local

dynamics at X^* is given to first-order by analyzing the eigenvalues of the Jacobian

$$J(X;\mu)|_{X=X^*} = (D_X F)(X^*;\mu) = \left(\frac{\partial F_i}{\partial X_j}(X^*;\mu)\right)_{ij}. \tag{4}$$

If we do not specify F exactly then X^* has to be treated as an unknown. The derivatives of functions/rates at the unknown equilibrium are often difficult to interpret in terms of physical parameters. Therefore we would like to consider a transformation that allows a physical interpretation of parameters. Generalized modeling [20] suggests to assume that $X_i^* \neq 0$ and to consider the `normalizing coordinate change`

$$x_i = \frac{X_i}{X_i^*} =: h_i(X), \qquad \text{for } i \in \{1,2,\ldots,n\}. \tag{5}$$

The ODE (1) transforms to

$$x_i' = \frac{1}{X_i^*} F_i(X_1^* x_1, X_2^* x_2, \ldots, X_n^* x_n) =: \tilde{F}_i(x), \qquad \text{for } i \in \{1,2,\ldots,n\} \tag{6}$$

where we have omitted the μ parameter dependence for notational convenience. Therefore the equilibrium X^* is transformed to $x^* = (1,1,\ldots,1) =: 1$.

Remark: A standard coordinate change in bifurcation theory [24] is to consider the transformation $\bar{x}_i := X_i - X_i^*$ so that the equilibrium point is moved to $\bar{x} = (0,\ldots,0) =: 0$. This transformation is mathematically convenient but does not provide a normalization of parameters as the coordinate change (5).

We can immediately check that the eigenvalues of the Jacobian (4) remain unchanged.

Proposition 2.2. *If $X_i^* \neq 0$ for all $i \in \{1,\ldots,N\}$ then the eigenvalues of the Jacobian are invariant under* (5) *i.e. spec$(D_X F(X^*)) =$ spec$(D_x \tilde{F}(1))$.*

Proof. By direct calculation we find that

$$\begin{aligned}
\det\left[(D_x\tilde{F})(1) - \lambda\,\mathrm{Id}\right] &= \det\left[\left(\frac{\partial}{\partial x_j}\frac{1}{X_i^*}F_i(X_1^*x_1, X_2^*x_2, \ldots, X_n^*x_n)\right)_{ij}\Bigg|_{x=1} - \lambda\,\mathrm{Id}\right] \\
&= \det\left[\left(\frac{X_j^*}{X_i^*}\frac{\partial F_i}{\partial X_j}(X^*) - \frac{X_j^*}{X_i^*}\lambda\delta_{ij}\right)_{ij}\right] \\
&\overset{(a)}{=} \left(\prod_{i=1}^n \frac{1}{X_i^*}\right)\det\left[\left(X_j^*\frac{\partial F_i}{\partial X_j}(X^*) - X_j^*\lambda\delta_{ij}\right)_{ij}\right] \\
&\overset{(b)}{=} \left(\prod_{j=1}^n X_j^*\right)\left(\prod_{i=1}^n \frac{1}{X_i^*}\right)\det\left[\left(\frac{\partial F_i}{\partial X_j}(X^*) - \lambda\delta_{ij}\right)_{ij}\right] \\
&= \det[(D_X F)(X^*) - \lambda\,\mathrm{Id}]
\end{aligned}$$

where we have factored out non-zero scalars in step (a) for each row and in (b) for each column using linearity of determinants with respect to rows and columns. The result follows. □

The equivalence of eigenvalues and the associated stability properties turns out to be of primary importance in many applications of generalized models [22]. However, Proposition 2.2 can also be viewed as a corollary to the following global result.

Proposition 2.3. *Suppose that $F \in C^k$ for some $k \in \mathbb{N}_0 \cup \{\omega\}$, where C^ω denotes analytic functions, and that $X_i^* \neq 0$. Then the ODEs* (1) *and* (6) *are C^k-smoothly equivalent via the map* (5).

Proof. Observe that $x = h(X) = (h_1(X), \ldots, h_n(X))$ is a C^k-diffeomorphism that conjugates the vector fields

$$F(X) = (D_X h)^{-1}(X)\ \tilde{F}(h(X)).$$

□

The global smooth equivalence we showed is much stronger than (local) topological equivalence [41] and the normalizing coordinate change (5) can be viewed as leaving the dynamics completely unchanged. The next steps of generalized modeling involves grouping and labeling the free parameters so that they can be interpreted as modeling parameters.

3 Parameters

We introduce a notation for the normalized gain and loss terms

$$f_{i,k}(x) := \frac{F_{i,k}(X_1^* x_1, \ldots, X_n^* x_n)}{F_{i,k}(X^*)} = \frac{F_{i,k}(X_1^* x_1, \ldots, X_n^* x_n)}{F_{i,k}^*} \tag{7}$$

where $F_{i,k}^* := F_{i,k}(X^*)$ and we assume that $F_{i,k}(X^*) \neq 0$. Then (6) reads

$$x_i' = \sum_{k=1}^{K_i} a_{i,k} \frac{F_{i,k}^*}{X_i^*} f_{i,k}(x), \qquad \text{for } i \in \{1, 2, \ldots, n\}. \tag{8}$$

As a next step we group two parameters together

$$\tilde{\beta}_{i,k} := \frac{F_{i,k}^*}{X_i^*}. \tag{9}$$

Remark: From a physical point of view, we can also consider the units in the definition of $\tilde{\beta}_{i,k}$. $F_{i,k}^*$ is always a rate, for example mass per unit time. Since X^* has also units of mass this implies that $\tilde{\beta}_{i,k}$ has the unit 1/time.

Using definition (9) and the equilibrium point condition $x_i' = 0$ at $x^* = 1$ in (8) gives n conditions

$$0 = \sum_{k=1}^{K_i} a_{i,k} \tilde{\beta}_{i,k} \qquad \text{for } i \in \{1, 2, \ldots, n\}. \tag{10}$$

Therefore we can hope to eliminate i parameters. For example, we could try to eliminate $\tilde{\beta}_{i,1}$ and set $\tilde{\beta}_{i,1} = a_{i,1}(-\sum_{a_{i,k}=1,k\neq 1}\tilde{\beta}_{i,k} + \sum_{a_{i,k}=-1}\tilde{\beta}_{i,k})$. We can formalize the elimination procedure as follows. Define the vector

$$\tilde{\beta} := (\tilde{\beta}_{1,1}, \tilde{\beta}_{1,2}, \ldots, \tilde{\beta}_{1,K_1}, \tilde{\beta}_{2,1}, \ldots, \tilde{\beta}_{n,K_n})^T \in \mathbb{R}^\kappa \tag{11}$$

where $\kappa = \sum_{i=1}^n K_i$. Then (10) can be re-written as a matrix equation

$$0 = \mathcal{A}\tilde{\beta} \tag{12}$$

where the $n \times \kappa$ matrix $\mathcal{A}$ has elements in $\{-1, 0, 1\}$; see also Example 3.2 below. The rank-nullity theorem gives

$$\kappa = \dim(\ker(\mathcal{A})) + \dim(\mathrm{im}(\mathcal{A})) = \dim(\ker(\mathcal{A})) + \mathrm{rank}(\mathcal{A})). \tag{13}$$

This shows that $\mathrm{rank}(\mathcal{A})$ is the number of parameters that we can eliminate and that $\dim(\ker(\mathcal{A}))$ is the number of remaining parameters after the linear relations (10) have been applied. The elimination of parameters is related to concepts used in structural kinetic modeling where the matrix $\mathcal{A}$ can be viewed as a stoichiometric reaction matrix with normalized entries [49, 31, 48].

Note that the choice which of the parameters $\tilde{\beta}_{i,k}$ we eliminate is mathematically equivalent. However, it could be of significant importance in applications if we can eliminate the parameter we know least about. A further optional step is to introduce a parameter α_i for each variable and set

$$\beta_{i,k} := \frac{\tilde{\beta}_{i,k}}{\alpha_i}. \tag{14}$$

where we assume that $\alpha_i > 0$.

Remark: From a physical point of view, we want to introduce α_i to `nondimensionalize`. This implies that α_i has to have the unit 1/time while $\beta_{i,k}$ is dimensionless; in this case, we can interpret $\beta_{i,k}$ as ratios. One particular important choice to make this interpretation more precise is to consider the possible definition [20]

$$\alpha_i := \sum_{k:\ a_{i,k}=1} \tilde{\beta}_{i,k} = \sum_{k:\ a_{i,k}=-1} \tilde{\beta}_{i,k} \tag{15}$$

where the equality between the two sums follows from (12). Using this definition we find that

$$\beta_{i,k} = \frac{\tilde{\beta}_{i,k}}{\sum_{k:\ a_{i,k}=1}\tilde{\beta}_{i,k}} = \frac{\tilde{\beta}_{i,k}}{\sum_{k:\ a_{i,k}=-1}\tilde{\beta}_{i,k}}$$

which interprets $\beta_{i,k}$ as the rate associated to the term with index (i,k) divided by the total gain (or loss) rate i.e. we have obtained a ratio; see also Section 6. We shall not make explicit use of definition (15) here as it can be viewed as one particular choice of nondimensionalization. One can define a `time scale` as a physical quantity that has units 1/time. Therefore we shall call α_i `time scale parameters` from now on. Note that this justifies

our assumption $\alpha_i > 0$ on the basis of the underlying physical process.

Now we can re-write the differential equation (8) as

$$x_i' = \alpha_i \left(\sum_{k=1}^{K_i} a_{i,k} \beta_{i,k} f_{i,k}(x) \right), \qquad \text{for } i \in \{1, 2, \ldots, n\} \tag{16}$$

where the relation (12) is understood to apply as well. We call the parameters α_i and $\beta_{i,k}$ (resp. $\tilde{\beta}_{i,k}$) `scale parameters`. Obviously we have introduced quite a number of scale parameters to avoid specifying the functions in our model; therefore it is important to know how many scale parameters will appear in the model. We have the following result:

Proposition 3.1. *The number of scale parameters for a generalized model* (8) *is as follows:*

(C1) If $\tilde{\beta}_{i,k}$ are the only scale parameters and $\tilde{\beta}_{i,k} \neq \tilde{\beta}_{l,m}$ for all pairs $(i,k) \neq (l,m)$ then the minimum number of scale parameters is given by

$$\kappa - \mathit{rank}(\mathcal{A}) = \dim(\mathit{ker}(\mathcal{A})). \tag{17}$$

If all $\tilde{\beta}_{i,k}$ appear as multiplicative factors after the elimination via $A\tilde{\beta} = 0$ then one more parameter can be eliminated.

(C2) If $\beta_{i,k}$, α_i are the scale parameters and $\beta_{i,k} \neq \beta_{l,m}$ for all pairs $(i,k) \neq (l,m)$ then the minimum number of scale parameters is

$$\dim(\mathit{ker}(\mathcal{A})) + n - \eta - 1 \tag{18}$$

where η is the number of scale parameters $\beta_{i,k}$ that appear as multiplicative pre-factors after the elimination via (12)*.*

Remark: If the conditions $\tilde{\beta}_{i,k} \neq \tilde{\beta}_{l,m}$ resp. $\beta_{i,k} \neq \beta_{l,m}$ are violated then further parameters can obviously be eliminated. However, a violation of this condition is not generic within the class of vector fields we consider here so we shall not consider this situation any further; for more on genericity see Section 4.

Proof. (of Proposition 3.1) The previous discussion leading up to equation (13) yields (17). The second part of (C1) that allows the elimination of one further parameter will be clear once we proved (C2). For (C2), we have $\dim(\ker(\mathcal{A}))$ parameters $\beta_{i,k}$ and n parameters α_i after using the linear relations $\mathcal{A}\beta = 0$. Assume without loss of generality that in the first η coordinates, the parameters $\beta_{1,k}, \ldots, \beta_{\eta,k}$ appear as multiplicative prefactors so that the ODEs are

$$\begin{aligned}
x_1' &= \alpha_1 \beta_{1,1} \textstyle\sum_{k=1}^{K_1} a_{1,k} f_{i,k}(x), \\
&\vdots \\
x_\eta' &= \alpha_\eta \beta_{\eta,1} \textstyle\sum_{k=1}^{K_1} a_{\eta,k} f_{\eta,k}(x), \\
x_{\eta+1}' &= \alpha_{\eta+1} \textstyle\sum_{k=1}^{K_1} \beta_{\eta+1,k} a_{\eta+1,k} f_{\eta+1,k}(x), \\
&\vdots \\
x_n' &= \alpha_n \textstyle\sum_{k=1}^{K_1} \beta_{n,k} a_{n,k} f_{n,k}(x),
\end{aligned} \tag{19}$$

Now we define new time scale parameters $\tilde{\alpha}_i := \alpha_i \beta_{i,k} = \tilde{\beta}_{i,k}$ for $i \in \{1, 2, \ldots, \eta\}$ and $\tilde{\alpha}_i = \alpha_i$ for $i \in \{\eta + 1, \ldots, n\}$ which transforms (19) to

$$\begin{array}{rcl} x_1' & = & \tilde{\alpha}_1 \sum_{k=1}^{K_1} a_{1,k} f_{i,k}(x), \\ & \vdots & \\ x_\eta' & = & \tilde{\alpha}_\eta \sum_{k=1}^{K_1} a_{\eta,k} f_{\eta,k}(x), \\ x_{\eta+1}' & = & \tilde{\alpha}_{\eta+1} \sum_{k=1}^{K_1} \beta_{\eta+1,k} a_{\eta+1,k} f_{\eta+1,k}(x), \\ & \vdots & \\ x_n' & = & \tilde{\alpha}_n \sum_{k=1}^{K_1} \beta_{n,k} a_{n,k} f_{n,k}(x). \end{array} \tag{20}$$

Therefore we have eliminated η additional parameters. To eliminate one more parameter we can choose one time scale parameter $\tilde{\alpha}_i$, say without loss of generality $\tilde{\alpha}_1$, and apply a time re-scaling

$$t \mapsto t/\tilde{\alpha}_1.$$

Defining new parameters $\tilde{\alpha}_i/\tilde{\alpha}_1$ yields the final result. □

We use the planar Example (2.1) to illustrate the elimination of parameters.

Example 3.2. We continue with equations (3) from Example 2.1. Applying the definitions of the scale parameters we find that

$$\begin{array}{rcl} x_1' & = & \alpha_1 \left(\beta_{1,1} f_{1,1}(x_1; \mu) - \beta_{1,2} f_{1,2}(x_1, x_2; \mu) \right) \\ x_2' & = & \alpha_2 \left(\beta_{2,1} f_{1,2}(x_1, x_2; \mu) - \beta_{2,2} f_{2,2}(x_2; \mu) \right) \end{array} \tag{21}$$

where we can immediately see from (12) that

$$\beta_{1,1} = \beta_{1,2} \qquad \text{and} \qquad \beta_{2,1} = \beta_{2,2}.$$

More formally we could also define the vector $\beta = (\beta_{1,1}, \beta_{1,2}, \beta_{2,1}, \beta_{2,2})$ as in (11). The linear system (12) is then defined by the matrix

$$\mathcal{A} = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix}.$$

Obviously we have $\kappa = 4$, $\text{rank}(\mathcal{A}) = 2$ and $\dim(\ker(\mathcal{A})) = 2$. Therefore the ODE (21) can also be written as

$$\begin{array}{rcl} x_1' & = & \alpha_1 \beta_{1,1} \left(f_{1,1}(x_1; \mu) - f_{1,2}(x_1, x_2; \mu) \right) \\ x_2' & = & \alpha_2 \beta_{2,1} \left(f_{1,2}(x_1, x_2; \mu) - f_{2,2}(x_2; \mu) \right) \end{array} \tag{22}$$

which shows that for just one gain and one loss term per variable the ODEs simplify considerably. As suggested in the proof of Proposition 3.1 we define

$$\tilde{\alpha}_i := \alpha_i \beta_{i,1}.$$

A time re-scaling $t \mapsto t/\tilde{\alpha}_1$ then gives

$$\begin{array}{rcl} x_1' & = & \left(f_{1,1}(x_1; \mu) - f_{1,2}(x_1, x_2; \mu) \right) \\ x_2' & = & \frac{\tilde{\alpha}_2}{\tilde{\alpha}_1} \left(f_{1,2}(x_1, x_2; \mu) - f_{2,2}(x_2; \mu) \right) \end{array} \tag{23}$$

and a re-labeling $\alpha := \frac{\tilde{\alpha}_2}{\tilde{\alpha}_1}$ reduces the situation to one parameter where α is a ratio of time scales.

We continue by interpreting the parameters $\beta_{i,k}$. They are gain and loss ratios for each term in the decomposition. To analyze the stability and bifurcations of the equilibrium $x^* = 1$ we define `elasticities` (or `exponent parameters`)

$$f_{i,k,x_j} := \frac{\partial f_{i,k}}{\partial x_j}(1) = \left.\frac{\partial f_{i,k}}{\partial x_j}(x)\right|_{x=1}$$

and find the Jacobian of (16) at $x = 1$

$$J(1) = \begin{pmatrix} \alpha_1 & 0 & \cdots & 0 \\ 0 & \alpha_2 & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & & \alpha_n \end{pmatrix} \begin{pmatrix} \sum_{k=1}^{K_1} a_{1,k}\beta_{1,k}f_{1,k,x_1} & \cdots & \sum_{k=1}^{K_1} a_{1,k}\beta_{1,k}f_{1,k,x_n} \\ \vdots & \ddots & \vdots \\ \sum_{k=1}^{K_n} a_{n,k}\beta_{n,k}f_{n,k,x_1} & \cdots & \sum_{k=1}^{K_n} a_{n,k}\beta_{n,k}f_{n,k,x_n} \end{pmatrix}. \quad (24)$$

We also refer to the set of scale and exponent parameters as `generalized parameters`.

Example 3.3. We continue with equations (21) from Example 3.2 without considering additional time scale parameters (i.e. we set $\alpha = 1$). The Jacobian at the equilibrium is then given by

$$J(1) = \begin{pmatrix} f_{1,1,x_1} - f_{1,2,x_1} & f_{1,2,x_2} \\ f_{1,2,x_1} & f_{1,2,x_2} - f_{2,2,x_2} \end{pmatrix} \quad (25)$$

which gives a total number of three generalized parameters.

The key input to the generalized modeling process from applications is that we can often interpret the scale parameters and the elasticities for a given application. To explain the term elasticities we examine their definition more closely and observe that

$$f_{i,k,x_j} = \frac{\partial f_{i,k}}{\partial x_j}(1) = \frac{X_j^*}{F_{i,k}(X^*)}\frac{\partial F_{i,k}}{\partial X_j}(X^*) = X_j^*\left(\frac{\partial}{\partial X_j}\ln F_{i,k}(X)\right)_{X=X^*} = \left(\frac{\partial}{\partial x_j}\ln f_{i,k}(x)\right)_{x=1}$$

which interprets the exponent parameters as (scaled) logarithmic derivatives. Logarithmic derivatives are often called elasticities, particularly in the context of modeling economic problems [10]. We can also view the exponent parameter f_{i,k,x_j} as the `sensitivity` to variations of $f_{i,k}$ in the direction x_j at the equilibrium point [47]. If certain specific functional forms $F_{i,k}(X)$ are known from the modeling process we can get even more information (see [15], p.49). We give a few examples using univariate functions $F_{i,k}(X)$ with $X \in \mathbb{R}$:

$F_{i,k}(X)$	$f_{i,k,x}$
AX^q	q
$A\exp(BX^q)$	qBX^*
$\frac{A}{B+X^q}$	$-q\left(\frac{(X^*)^q}{B+(X^*)^q}\right)$
$\frac{AX^p}{B+X^q}$	$\frac{(B+(X^*)^p)(Bp+(p-q)(X^*)^q)}{(B+(X^*)^q)^2}$

Further possible dependencies of the exponent parameters are easily derived by direct differentiation of the given functional form.

4 Bifurcations

Using the $n \times n$ Jacobian matrix (24) we have access to the eigenvalues and their multiplicities at the equilibrium point $x = 1$ ($X = X^*$). One can calculate the eigenvalues λ_i numerically using standard methods such as unsymmetric QR factorization [13]. If $\Re(\lambda_i) \neq 0$ for all $i \in \{1, 2, \ldots, n\}$ the Hartman-Grobman Theorem [29] implies that the flow near $x = 1$ is locally topologically equivalent to the flow of the linearized system. In particular, we get asymptotic stability if $\Re(\lambda_i) < 0$ for all i. Therefore a necessary condition for bifurcation under parameter variation is that $\Re(\lambda_i) = 0$ for one (or multiple) eigenvalues. We briefly recall how to define an unfolding of a generic bifurcating family [56, 2] as we need this terminology throughout this section. Let $F \in C^r(\mathbb{R}^n, \mathbb{R}^n)$ be a vector field defining the ODE (1). The smoothness r will not be of primary relevance for us and we always assume that r is sufficiently large in the following. Let $J^s_x(F)$ denote the s-jet

$$(x, F(x), DF(x), D^2F(x), \ldots, D^sF(x))$$

of F at x with $s \leq r$; denote the associated space of jets by $J^s(\mathbb{R}^n, \mathbb{R}^n)$. The s-jet extension $\hat{F}$ of F is a map

$$\hat{F} : \mathbb{R}^n \to J^s(\mathbb{R}^n, \mathbb{R}^n), \qquad \hat{F}(x) = J^s_x(F)$$

that maps a phase space point to the associated jet; observe that we can identify the jet space $J^s(\mathbb{R}^n, \mathbb{R}^n)$ with $\mathbb{R}^m$ for a suitable m. Let $x_0 \in \mathbb{R}^n$ denote a phase space point and let U be a neighborhood of x_0 and set $V := F(U)$; we shall restrict to studying the local behavior of the vector field near x_0 from now on. Let $\mathcal{E} \subset J^s(U, V)$ denote the codimension n subset of those s-jets that have an equilibrium point x_0 in U [56] where codimension is defined as

$$\operatorname{codim}(\mathcal{E}) = \dim(J^s(U, V)) - \dim(\mathcal{E}) = m - \dim(\mathcal{E}).$$

Let $\mathcal{B} \subset \mathcal{E} \subset J^s(U, V)$ denote the codimension $n+1$ set of vector fields with a non-hyperbolic equilibrium point x_0; observe that a non-hyperbolic equilibrium point is defined by conditions on $DF(x_0)$. Consider an s-jet $J^s_x(F)$ with a non-hyperbolic equilibrium point at x_0. Then $J^s_x(F)$ lies in a set $\mathcal{D} \subseteq \mathcal{B}$ of codimension b in $J^s(U, V)$ for $b \geq n + 1$ and we define the codimension of the equilibrium point x_0 as $b - n$. To understand the dynamics near a bifurcation point in $\mathcal{D}$ we need a parameterized family of vector fields $F(x; \mu)$ so that the associated family of s-jets is transverse to $\mathcal{D}$. Recall that transversality of maps $G \in C^r(\mathbb{R}^n, \mathbb{R}^m)$ to a submanifold $M \subset \mathbb{R}^m$ at $G(x_0)$ is defined by the requirement

$$DG(x_0)T_{x_0}\mathbb{R}^n + T_{G(x_0)}M = T_{G(x_0)}\mathbb{R}^m.$$

The following theorem is of fundamental importance to justify the next steps. To state the theorem we recall that a property that holds for a countable intersection of dense open sets (i.e. on a residual set) is called generic.

Theorem 4.1 (Thom's Transversality Theorem, [42])**.** *Let M be a submanifold of $J^s(U, V)$. The set of maps $F \in C^r(U, V)$ whose s-jet extensions are transversal to M is a residual set in $C^r(U, V)$ (for some r depending on s and n).*

Hence if we can find a parameterized family $F(x;\mu)$ with $\mu \in \mathbb{R}^p$ which is transverse to $\mathcal{D}$ then we have constructed a generic representative. However, so far we have not taken the dynamics completely into account. Consider a vector field F^* with $F^*(x_0, \nu_0) = 0$. We say that $F^*(x,\nu)$ is induced from $F(x,\mu)$ near (x_0,μ_0) if there is a continuous map ϕ, defined near μ_0 with $\phi(\nu_0) = \mu_0$, so that

$$F^*(x,\nu) = F(x,\phi(\nu)).$$

A parameterized family $F(x,\mu)$ is called a universal unfolding near an equilibrium point (x_0,μ_0) if every other parameterized family of C^r vector fields is equivalent to a family of vector fields induced by $F(x,\mu)$. In general, it is difficult to verify for many bifurcations with higher-dimensional parameter spaces that a transversal family also forms a universal unfolding.

Remark: Although the results described so far give a framework for the classification of bifurcation points according to codimension there are a few subtle technical points regarding e.g. the applicability of Thom's Theorem 4.1 or possible re-parameterizations of time and coordinate changes [56].

The classification of local bifurcation according to codimension [41, 24] yields the following classification up to codimension two:

- *codim* = 1: Fold or saddle-node (single zero eigenvalue), Hopf (pair of pure imaginary eigenvalues).
- *codim* = 2: Bogdanov-Takens (double real zero eigenvalues), Gavrilov-Guckenheimer or fold-Hopf (single zero eigenvalue and pure imaginary pair of eigenvalues), Hopf-Hopf (two pairs of pure imaginary eigenvalues), cusp (single zero eigenvalue and degenerate normal form coefficient), Bautin or generalized Hopf (pair of pure imaginary eigenvalues and zero first Lyapunov coefficient).

The eigenvalues of (24) depend on the generalized parameters so that we can detect necessary conditions for all codimension one and two bifurcations except cusp and Bautin bifurcation that are of codimension two as they violate codimension one non-degeneracy conditions. We shall not aim at a complete discussion of bifurcation analysis of generalized models but point out some features via examples.

Example 4.2. Consider the following generalized toy model

$$X' = F_1(X) - F_2(X) + F_3(X) \tag{26}$$

for $X \in \mathbb{R}$. A possible specific model covered by (26) is

$$X' = X^2 - 2X + 1 - A, \qquad \text{for } A \in (-1,1) \tag{27}$$

where $F_1(X) = X^2$, $F_2(X) = 2X$ and $F_3(X) = 1 - A$. It is easily checked that (27) has two equilibria at $X^*_\pm = 1 \pm \sqrt{A}$ for $A > 0$ that undergo a non-degenerate fold bifurcation

at $A = 0$. The bifurcation diagram is shown in Figure 1(a). After the normalizing scaling transformation $X = X^*_\pm x$ we find that (27) gives two ODEs

$$x' = X^*_\pm x^2 - 2x + \frac{1-A}{X^*_\pm} =: b_\pm(x, A), \qquad \text{for } A \in [0, 1). \tag{28}$$

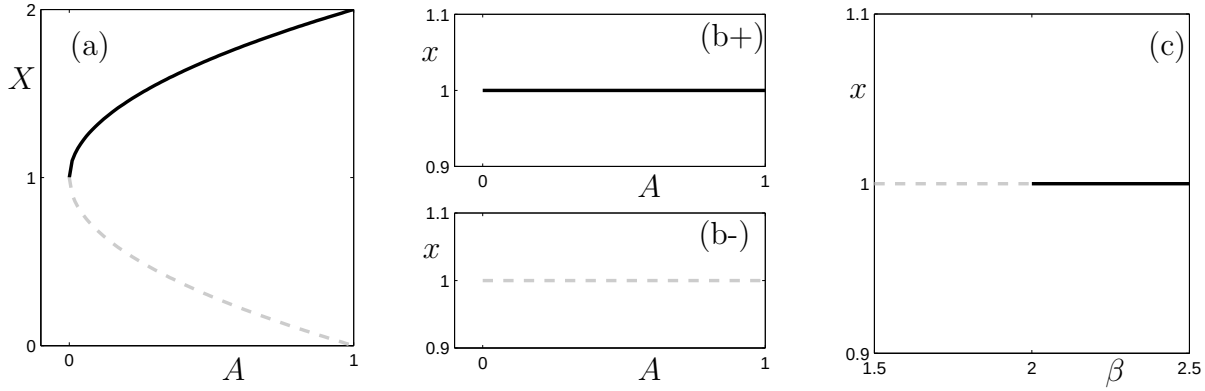

Figure 1: Solid black curves are stable equilibria and dashed grey curves unstable equilibria. (a) Fold bifurcation for the specific model (26). (b) Fold bifurcation for the re-scaled equations (28); we plotted the two equilibrium curves at $x = 1$ separately to indicate that they are associated to different branches in (a). (c) Bifurcation diagram for the generalized model (26).

The new bifurcation diagram of (28) is given in Figure 1(b±). The fold bifurcation from Figure 1(a) can still be recognized in Figure 1(b±) at $A = 0$ since

$$\frac{\partial b_\pm}{\partial x}(1, 0) = 0 \quad \text{and} \quad \frac{\partial^2 b_\pm}{\partial x^2}(1, 0) = 2.$$

The transversality condition requires looking at the parameter derivative

$$\frac{\partial b_\pm}{\partial A}(x, A) = \pm\frac{x^2 - 1}{2\sqrt{A}} \tag{29}$$

and we observe that the condition is not well-defined for $(x, A) = (1, 0)$. The generalized formulation of (26) is

$$x' = \alpha(\beta_1 f_1(x) - \beta_2 f_2(x) + (\beta_2 - \beta_1) f_3(x)). \tag{30}$$

Using a time re-scaling $t \mapsto t/(\alpha\beta_1)$ and setting $\beta := \beta_2/\beta_1$ we get that (30) can be written as

$$x' = f_1(x) - \beta f_2(x) + (\beta - 1) f_3(x). \tag{31}$$

The associated Jacobian for (31) at $x = 1$ is

$$J(1) = f_{1,x} - \beta f_{2,x} + (\beta - 1) f_{3,x}.$$

If we assume that the exponent parameters are $(f_{1,x}.f_{2,x}, f_{3,x}) = (2, 1, 0)$ as for our specific model then we find that

$$J(1) = 2 - \beta$$

which satisfies the necessary condition for a saddle-node bifurcation at $\beta = 2$. Since (30) always has an equilibrium point at $x = 1$ we find a bifurcation diagram as shown in Figure 1(c).

From Example 4.2 we conclude that a generalized model will be able to detect the main bifurcation conditions for eigenvalue crossings but that one has to be careful in interpreting bifurcation diagrams. Furthermore, a first-order analysis will not check whether non-degeneracy and transversality conditions are satisfied. This raises the issue of genericity for generalized models which we address in the next example.

Example 4.3. We continue with Example 4.2 and the generalized model

$$x' = f_1(x) - \beta f_2(x) + (\beta - 1)f_3(x) =: g(x, \beta). \tag{32}$$

We check the generalized model for genericity near a fold bifurcation. Consider the associated 1-jet space $J^1_x(\mathbb{R}, \mathbb{R})$ to g with elements

$$\left(x, g(x, \beta), \frac{\partial g}{\partial x}(x, \beta)\right)$$

which is three-dimensional. The bifurcation set $\mathcal{B}$ for a fold bifurcation is given by

$$\{(x, 0, 0) \in J^1_x(\mathbb{R}, \mathbb{R})\}$$

which has dimension 1 and codimension $b = 2$. Therefore we get, as expected, that the fold bifurcation has codimension $b - n = 2 - 1 = 1$. The 1-jet extension to $g : \mathbb{R} \to \mathbb{R}$ is the map

$$\hat{g}(x, \beta) = \left(x, g(x, \beta), \frac{\partial g}{\partial x}(x, \beta)\right) \tag{33}$$

which we view as a map from $\hat{g} : \mathbb{R}^2 \to \mathbb{R}^3$ including the generalized parameter β. The linearization of the 1-jet extension is

$$D\hat{g}(x, \beta) = \begin{pmatrix} 1 & 0 \\ \frac{\partial g}{\partial x}(x, \beta) & \frac{\partial g}{\partial \beta}(x, \beta) \\ \frac{\partial^2 g}{\partial x^2}(x, \beta) & \frac{\partial^2 g}{\partial x \partial \beta}(x, \beta) \end{pmatrix} \tag{34}$$

The tangent space to $\mathcal{B}$ is spanned by the vector $(1, 0, 0)^T \in T_{\hat{g}(x,\beta)}\mathbb{R}^3$; note that we can obviously identify $T_{\hat{g}(x,\beta)}\mathbb{R}^3$ with $\mathbb{R}^3$. Evaluating (34) at a fold bifurcation point $(1, \beta_0)$ we know that

$$\frac{\partial g}{\partial x}(1, \beta_0) = 0.$$

This implies that checking transversality of the 1-jet extension (33) reduces to checking that the 3×3 matrix

$$H := \begin{pmatrix} 1 & 0 & 1 \\ 0 & \frac{\partial g}{\partial \beta}(1, \beta_0) & 0 \\ \frac{\partial^2 g}{\partial x^2}(1, \beta_0) & \frac{\partial^2 g}{\partial x \partial \beta}(1, \beta_0) & 0 \end{pmatrix}$$

is non-singular. This just means

$$\det(H) = -\frac{\partial g}{\partial \beta}(1, \beta_0) \cdot \frac{\partial^2 g}{\partial x^2}(1, \beta_0) \neq 0.$$

This recovers the well-known [41] non-degeneracy conditions

$$\frac{\partial g}{\partial \beta}(1, \beta_0) \neq 0 \qquad \text{and} \qquad \frac{\partial^2 g}{\partial x^2}(1, \beta_0) \neq 0. \tag{35}$$

Recall that if (35) holds then the unfolding is indeed universal in β [24, 41]. Only the last step of the genericity analysis has to be adapted to the generalized model. In particular, we can plug in the structure of the model (32) into (35) which yields the conditions

$$\begin{array}{rcl} \frac{\partial g}{\partial \beta}(1, \beta_0) & = & -f_2(1) + f_3(1) \neq 0, \\ \frac{\partial^2 g}{\partial x^2}(1, \beta_0) & = & \frac{\partial^2 f_1}{\partial x^2}(1) - \beta_0 \frac{\partial^2 f_2}{\partial x^2}(1) + (\beta_0 - 1)\frac{\partial^2 f_3}{\partial x^2}(1) \neq 0. \end{array} \tag{36}$$

The conditions (36) restrict the function space for which one can expect that the generalized model has a fold bifurcation with a universal unfolding. The examples have also demonstrated that known results about bifurcations and unfoldings carry over easily to generalized models.

Even if the unfolding is not universal (e.g. if we had chosen a function space in Example (4.3) with $f_2(1) = f_3(1)$) then we can often use the availability of additional parameters as the next example illustrates.

Example 4.4. Consider a planar generalized model

$$\begin{array}{rcl} x_1' & = & \sum_{k=1}^{K_1} a_{1,k}\beta_{1,k} f_{1,k}(x), \\ x_2' & = & \sum_{k=1}^{K_2} a_{2,k}\beta_{2,k} f_{2,k}(x), \end{array} \tag{37}$$

where we assume that the time scales are all equal to 1 for simplicity. Suppose (37) has a Hopf bifurcation at $(x, \beta_{1,1}) = (1, \beta_{1,1}^*)$ so that the Jacobian $J(1)$ has a complex conjugate pair of eigenvalues. There are two non-degeneracy conditions [41]. The transversality condition is

$$f_{1,1}(1) \neq 0. \tag{38}$$

This condition is generically satisfied if we let $f_{1,1} \in C^r(\mathbb{R}^2, \mathbb{R})$ for some fixed $r \geq 0$; indeed, in this case maps $f_{1,1}$ that satisfy (38) form a residual set in the C^r topology. The second non-degeneracy condition is that the first Lyapunov coefficient l_1 is not equal to zero [40]. The condition can be written in terms of the partial derivatives with respect to $x_{1,2}$ up to third order. The scale parameters $\beta_{1,k}$ or $\beta_{2,k}$ appear as coefficients in the linear combination as they are multiplicative prefactors. Therefore we have $l_1 \neq 0$ generically in a sufficiently large space of scale parameters i.e. we obtain conditions analogous to (36) but with additional parameters. Hence additional generalized parameters can often compensate for a restricted choice of functions $f_{j,k}$.

The previous two examples illustrate the main aspects of the genericity question for generalized models:

1. We can check for a given decomposition and given function spaces whether the non-degeneracy conditions for a bifurcation are satisfied.

2. The checking depends crucially on the underlying mathematical modeling and how the functions and decomposition are chosen.

3. Higher-order terms have to be taken into account that are not parameterized by scale parameters and elasticities; see also [59].

We have seen that the scale parameters are relatively easy to understand. The elasticities are bit more complicated as the next example illustrates.

Example 4.5. In principle, we can also just vary the elasticities and treat them as bifurcation parameters. The obvious caveat is that this might not yield a smooth family of functions everywhere in phase space. For example, if

$$F_{i,k}(X) = A(X - B)^p, \qquad \text{for } p > 0 \tag{39}$$

where A, B are parameters, then $F_{i,k}$ is C^∞ for $X \neq B$ but only C^k for some finite k if $p \notin \mathbb{N}$. This can again lead to violations of non-degeneracy conditions for bifurcations as in Example (4.2). In particular, as shown in [39], we will not be able to conclude quantitative universal scaling laws near bifurcations if we do not restrict the functions $F_{i,k}$ to be sufficiently smooth. Note that this phenomenon is again non-generic for a sufficiently large parameter space. The second key observation for elasticities relates to the form of $f_{i,k}$. For (39) we find

$$f_{i,k,x} = \frac{pX^*}{X^* - B} \tag{40}$$

which depends on the equilibrium point location X^*. The best way to interpret (40) is asymptotic knowledge about X^*; for example, we have

$$\begin{array}{lll} X^* \gg 1, \quad B = O(1) & \Rightarrow & f_{i,k,x} \approx p, \\ X^* \approx B, \quad X^* = O(1) & \Rightarrow & f_{i,k,x} \gg 1, \\ 0 < X^* \ll 1, \quad B = O(1) & \Rightarrow & f_{i,k,x} \approx 0. \end{array}$$

where $O(1)$ indicates a fixed constant independent of any asymptotic limits of X^*.

The last example shows that it can be beneficial to restrict the class of functions considered in a generalized model to a certain class, e.g. smooth functions, polynomials or certain functionals particular to the application area [15]. The important conclusion of all previous examples is that generalized models produce information that "scales with the input". The more knowledge from the modeling process is available, the more detailed information about the dynamics can be derived.

We conclude this section by mentioning an important practical issue. We have to address how to find bifurcations and their associated varieties (such as surfaces, lines, curves, etc.) in parameter space. A direct method calculates the eigenvalues and uses iteration to find the zeros of real parts. An indirect method employs so-called test functions that vanish

once a certain type of eigenvalue crossing occurs; see [14] or [41] for an overview of different test functions and references to the literature. We note that analytical methods such as the method of resultants [26, 25] have also been employed successfully in the context of generalized modeling [20] using computer algebra [19]; having an explicit formula for the bifurcation loci can be beneficial for visualization [51]. Section 6.2 illustrates the search for bifurcations in generalized models with an example.

5 Beyond ODEs

Although we presented the ideas of generalized modeling only in the context of ODEs so far, it is evident that their scope is much broader. Recall that the key ideas are:

- There exist unknown functional forms in the model.
- Group the different parts of the vector field into gain and loss terms.
- Introduce a normalizing coordinate change for an equilibrium point.
- Re-scale the gain and loss terms and introduce scale parameters.
- Linearize at the new equilibrium $x = 1$ and introduce elasticities.
- Interpret the generalized parameters and assign suitable ranges.
- Use tools from bifurcation analysis to capture the dynamics.

These ideas carry over naturally into a much wider setup than just ODEs. Generalized models for discrete dynamical systems (iterated maps) are discussed in [38]. Many other mathematical evolution equations are very similar to ODEs. In particular, the notion of equilibrium point, coordinate changes or re-scaling as well as linearized analysis carry over. In this section we shall demonstrate this observation for certain classes of partial, functional and stochastic differential equations.

5.1 Partial Differential Equations

We have seen in Section 2 that generalized models provide a tool to analyze the dynamics of ordinary differential equations. A class of partial differential equations (PDEs) that can be analyzed by dynamical systems techniques is given by (semilinear) parabolic equations. Let $(x,t) \in \Omega \times \mathbb{R}^+$ where $\Omega \subset \mathbb{R}^n$ is a domain and let $u = u(\cdot,t) \in X$ for all $t \geq 0$ where X is a suitable Banach space e.g. $X = L^p(\Omega)$; for details see [32]. Consider the abstract evolution equation

$$\frac{\partial u}{\partial t} + Au = F(x,t,u;\mu) \tag{41}$$

where $F : \Omega \times \mathbb{R}^+ \times X \times \mathbb{R}^p \to \mathbb{R}^n$ and A is a sectorial (differential) operator on X [32]. A concrete example for (41) are initial boundary value problems for reaction-diffusion PDEs

[35] of the form

$$\begin{array}{rcll} \frac{\partial u}{\partial t} - \mathcal{D}\Delta u &=& F(x,t,u;\mu) & \text{for } x \in \Omega,\, t > 0 \\ u(x,t) &=& g(x,t) & \text{for } x \in \partial\Omega,\, t > 0 \\ u(x,0) &=& h(x) & \text{for } x \in \partial\Omega \end{array} \tag{42}$$

for $g : \Omega \times \mathbb{R}^+ \to \mathbb{R}^n$, $h : \Omega \to \mathbb{R}^n$, Δ is the Laplacian and $\mathcal{D}$ is a diagonal matrix called the diffusion matrix with non-negative elements. We shall restrict our presentation of generalized models here to (42) but remark that the ideas naturally extend to many other equations within the class (41). Assume that F can again be decomposed into gain and loss terms

$$F_i(u,x,t) = \sum_{k=1}^{K_i} a_{i,k} F_{i,k}(u,x,t).$$

where we omit the parameters $\mu \in \mathbb{R}^p$ again for notational convenience. Note that this assumption is very natural in the context of reaction-diffusion systems since F represents the reaction terms. For example, if we think of a chemical reaction then gain terms would be terms that increase a concentration while loss terms decrease it. Suppose (42) there exists a constant function u^* such that

$$u^*(x,t) = (u_1^*, \ldots, u_n^*), \qquad , \qquad u_i^* \in \mathbb{R}, \quad u_i^* \neq 0,$$

for all $t > 0$. Then u^* is a space-time homogeneous equilibrium solution to (42). We can apply the normalizing coordinate change

$$v_i := \frac{u_i}{u_i^*}, \qquad \text{for } i \in \{1, 2, \ldots, n\}.$$

Then the reaction-diffusion system (42) transforms to

$$\begin{array}{rcll} \frac{\partial v_i}{\partial t} - \alpha_i \tilde{\mathcal{D}}_{ii}\Delta v_i &=& \frac{F_i(x,t,v_1 u_1^*,\ldots,v_n u_n^*)}{u_i^*} =: \alpha_i \sum_{k=1}^{K_i} a_{i,k}\beta_{i,k} f_{i,k}(x,t,v), & x \in \Omega,\, t > 0 \\ v_i(x,t) &=& \frac{g_i(x,t)}{u_i^*} =: g_i^*(x,t), & x \in \partial\Omega,\, t > 0 \\ v_i(x,0) &=& \frac{h_i(x)}{u_i^*} =: h_i^*(x), & x \in \partial\Omega \end{array} \tag{43}$$

where the usual generalized modeling definitions as in (16) are used and the diffusion matrix has been rescaled $\tilde{\mathcal{D}}_{ii} = \mathcal{D}_{ii}/\alpha_i$. Then (43) has a space-time homogeneous equilibrium at $v = (1, 1, \ldots, 1) =: 1$. Now all linearization techniques at $v = 1$ for (43) can make use of the interpretation of scale parameters and elasticities as before. As a typical example one can consider the Turing-Hopf mechanism [35]. Let $J(1)$ denote the Jacobian as in (24). If $J(1)$ has only eigenvalues $\lambda = \lambda(k)$ with $\Re(\lambda) < 0$ then the equilibrium $v = 1$ is stable as a solution to $v' = J(1)v$. The Turing-Hopf bifurcation requires that some eigenvalue of the Laplacian has $\Re(\lambda(k)) > 0$ for some $k \geq 1$ which results in a spatial instability and associated pattern formation. Explicit conditions for this scenario to occur can then be derived in terms of the generalized parameters and the rescaled diffusion coefficients [4].

5.2 Delay Differential Equations

Consider a delay differential equation (DDE) with constant delays t_l, $l \in \{1, 2, \ldots, m\}$, given by

$$X' = F(X(t), X(t-\tau_1), X(t-\tau_2), \ldots, X(t-\tau_m); \mu) \tag{44}$$

where $F : \mathbb{R}^{(m+1)n} \times \mathbb{R}^p \to \mathbb{R}^n$ and we abbreviate $X(t-\tau_l)$ as X^{τ_l}; see also [33]. As for PDEs, we remark that (44) only presents a subclass of DDEs as it is non-neutral with constant delays [28] and we expect generalized modeling to apply for many more DDEs than just (44). Suppose there exists an equilibrium point $X = X^*$ so that

$$F(X^*, X^*, \ldots, X^*; \mu) = 0.$$

Applying the usual generalized modeling procedure we end up with

$$x_i' = \alpha_i \left(\sum_{k=1}^{K_i} a_{i,k} \beta_{i,k} f_{i,k}(x) \right) \tag{45}$$

where the scale parameters are defined as usual and

$$f_{i,k}(x) = \frac{F_{i,k}(X^* \cdot x, X^* \cdot x^{\tau_1}, \ldots, X^* \cdot x^{\tau_n})}{X_i^*}.$$

The linearized equation for (45) around $x = 1$ is

$$v' = \sum_{l=0}^{m} A_l v^{\tau_l} \tag{46}$$

where the $n \times n$ matrices A_l consists of the rows

$$\alpha_i \left(\sum_{k=1}^{K_i} a_{i,k} \beta_{i,k} \sum_{l=0}^{m} (D_l f_{i,k})(1) \right)$$

and where D_l denotes the total derivative of $f_{i,k}$ with respect to the l-th argument; note that we have employed the convention $\tau_0 = 0$ so that $l = 0$ denotes the first argument. The characteristic equation associated to (46) is obtained by assuming an exponential solution of the form $e^{\lambda t}$ and is given by

$$\det \left(\lambda \mathrm{Id} - \sum_{l=0}^{m} e^{-\lambda \tau_l} A_l \right) = 0. \tag{47}$$

In contrast to ODEs, we see that (47) is a transcendental equation which can have an infinite number of solutions λ. It is known that if $\Re(\lambda) < 0$ for every solution then the solution is stable. Bifurcation analysis for (47) can then be carried out using numerical [7] or analytical [9] methods. The generalized parameters are used as bifurcation parameters in this context.

5.3 Stochastic Differential Equations

Consider a system of stochastic differential equations (SDEs) [43]

$$dX = F(X; \mu)dt + G(X; \mu)dW \tag{48}$$

where $W = W(t) = (W_1(t), W_2(t), \ldots, W_k(t))^T$ is a k-dimensional Brownian motion, $F : \mathbb{R}^n \to \mathbb{R}^n$, $G : \mathbb{R}^n \to \mathbb{R}^{n \times k}$ is a matrix-valued function. The normalizing coordinate change

(5) can be applied to (48) for a deterministic equilibrium $F(X^*) = 0$ with $X_i^* \neq 0$ for all $i \in \{1, \ldots, n\}$. Since the coordinate change is linear the Itô formula [11, 37] reduces to the standard chain rule and we get

$$dx_i = \frac{F_i(X_1 x_1, \ldots, X_n x_n; \mu)}{X_i^*} dt + \frac{1}{X_i^*} G_i(X_1 x_1, \ldots, X_n x_n; \mu) dW, \quad \text{for } i \in \{1, 2, \ldots, n\}$$

where G_i indicates the i-th row of G. The scale and exponent parameters for the deterministic drift terms $F_i(X; \mu)/X_i^*$ can be defined as in Section 3. We can also consider a normalized matrix-valued function for the diffusion term where each row is given by

$$g_i(x; \mu) := \frac{G_i(X_1 x_1, \ldots, X_n x_n; \mu)}{X_i^*}.$$

Then we can still formally linearize (48) at $x = 1$ and obtain to lowest order

$$d\xi = \left(\frac{\partial}{\partial x_j} \sum_{k=1}^{K_i} f_{i,k}(x; \mu) \bigg|_{x=1} \right)_{i,j} \xi dt + g(1; \mu) dW \tag{49}$$

where $\xi = \xi(t)$ now solves an SDE with linear drift term and constant diffusion. There are multiple possibilities on how to develop a "stochastic bifurcation theory" [34, 1]. Therefore we shall not discuss generalized modeling for SDEs in any more detail. However, we expect generalized models for SDEs to work for bifurcation and stability analysis as well.

6 Applications

In this section we briefly outline some of the applications of generalized modeling and highlight some of the major results. A comprehensive list of references for other applications is [20, 21, 22, 4, 52, 58, 51, 55, 18, 17, 16, 33, 49, 48, 57, 45, 3, 12]. For each example we focus on a different aspect of generalized modeling. In Section 6.1 we explain how to interpret the generalized parameters. In Section 6.2 we consider a generalized model for epidemics and illustrate how the computation of bifurcation surfaces in parameter space can be used for analysis. In Section 6.3 we illustrate the importance of equilibrium stability and how sampling-based methods can be used to understand large classes of mathematical models.

6.1 Dynastic Cycles

One problem considered in [20] describes the periodic behavior in a socio-economic setup with a focus on the transitions between despotism and anarchy that are called dynastic cycles [54]. The society is assumed to consist of farmers X, bandits Y and rulers Z. The ODEs are

$$\begin{aligned} X' &= S(X) - C(X, Y) - T(X, Z) \\ Y' &= \eta C(X, Y) - L(Y, Z) - M(Y) \\ Z' &= \nu C(X, Y) - R(Z) \end{aligned} \tag{50}$$

where $S(X)$ is growth of the farmer population, $C(X, Y)$ is loss due to crime, $T(X, Z)$ is loss due to taxes, $L(Y, Z)$ is the loss of bandits due to ruler intervention, $M(Y)$ is loss of bandits

due to mortality or retirement and $R(Z)$ is the loss of rulers due to the same factors. The generalized model associated with (50) can be written as

$$\begin{aligned} x' &= \alpha_x(s(x) - \beta_{1,2}c(x,y) - \beta_{1,3}t(x,z)) \\ y' &= \alpha_y(c(x,y) - \beta_{2,2}l(y,z) - \beta_{2,3}m(y)) \\ z' &= \alpha_z(c(x,y) - r(z)) \end{aligned} \tag{51}$$

where the functions have been normalized as in (7) and the parameters are given by

$$\alpha_x := \frac{S^*}{X^*}, \qquad \alpha_y := \frac{\eta C^*}{Y^*}, \qquad \alpha_z := \frac{\nu C^*}{Z^*}$$

and

$$\beta_{1,2} := \frac{C^*}{S^*}, \qquad \beta_{1,3} := \frac{T^*}{S^*}, \qquad \beta_{2,2} := \frac{L^*}{\eta C^*}, \qquad \beta_{2,3} := \frac{M^*}{\eta C^*}.$$

As examples for the interpretation of the scale parameters we consider $\beta_{1,3}$ and $\beta_{2,2}$. The parameter $\beta_{1,3}$ describes the ratio of loss of farmers via taxes in comparison to their natural growth/birth process. Alternatively we can also write $\beta_{1,3} = T^*/S^* = T^*/(\alpha_x X^*)$ which interprets $\beta_{1,3}$ as the loss due to taxes per unit time normalized by the total number of farmers. The parameter $\beta_{2,2}$ can be interpreted as the probability that a bandit is caught before reaching retirement age. Similar interpretations can be found for the other scale parameters and this allows us to assign the parameters ranges of values. The elasticities are defined as

$$s_x := \frac{\partial s}{\partial x}(1), \qquad c_y := \frac{\partial c}{\partial y}(1,1), \qquad \text{etc.}$$

We can interpret s_x as the sensitivity of the farmer's growth rate with respect to their number in the steady state. If land is available in abundance then the growth rate could be modeled as some linear function and we get $s_x = 1$. However, if the growth rate is entirely determined by the availability of land then the growth rate is completely insensitive to the number of farmers and we would get $s_x = 0$. Similar considerations can be used to interpret all the elasticities. Using a standard bifurcation analysis [20] one finds that one of the main bifurcation parameter that determines the stability of the system (51) is s_x and that a limited availability of land promotes stability. Stability of the equilibrium can be lost under the variation of s_x in a Hopf bifurcation that leads to dynastic cycles

6.2 Epidemics

Consider a classical two-component predator-prey model with predator population Y and prey population X. In [50, 53] the dynamics of this system is analyzed under the assumption that the predator suffers from an epidemic with SIRS dynamics. The model is given as follows

$$\begin{aligned} X' &= SX - G(X)(Y_S + Y_R + \alpha Y_I) - M_X X^2 \\ Y_S' &= EG(X)(Y_S + Y_R + \alpha\beta Y_I) - M_Y Y_S + \delta Y_R - \Lambda(Y_S, Y_I) \\ Y_I' &= \Lambda(Y_S, Y_I) - (M_Y + \mu)Y_I - \gamma Y_I \\ Y_R' &= \gamma Y_I - \delta Y_R - M_Y Y_R \end{aligned} \tag{52}$$

where Y_S, Y_I and Y_R are susceptible, infected and recovered predators. Note that (52) has some unknown functional forms such as the incidence/interaction $\Lambda(Y_S, Y_I)$ between the

susceptible and infected parts of the population. The equations also contain some specific functions such as $M_X X^2$ which describes the limiting growth factor of the prey due to intraspecific competition. The generalized model for (52) can be written, using the notation of [50, 53], as

$$\begin{aligned} x' &= \alpha_x[x-(1-m_x)g(x)((1-f_\alpha)(by_s+(1-b)y_r)+f_\alpha y_i)-m_x x^2] \\ y_S' &= \alpha_s[e_s g(x)((1-f_\beta)(by_s+(1-b)y_r)+f_\beta y_i) \\ &\quad -m_y y_s+(1-e_s)y_r-(1-m_y)l(y_s,y_i)] \\ y_I' &= \alpha_i[l(y_s,y_i)-y_i] \\ y_R' &= \alpha_r[y_i-y_r] \end{aligned} \tag{53}$$

where $\alpha_{x,s,i,r}$ are time scales and b, f_α, f_β, e_s, m_x, m_y are scale parameters. We also define

$$g_x := \frac{\partial g}{\partial x}(1), \qquad l_i := \frac{\partial l}{\partial y_i}(1,1), \qquad l_i := \frac{\partial l}{\partial y_i}(1,1)$$

as exponent parameters. The bifurcation conditions for (53) with respect to eigenvalues of $J(1)$ can then be investigated.

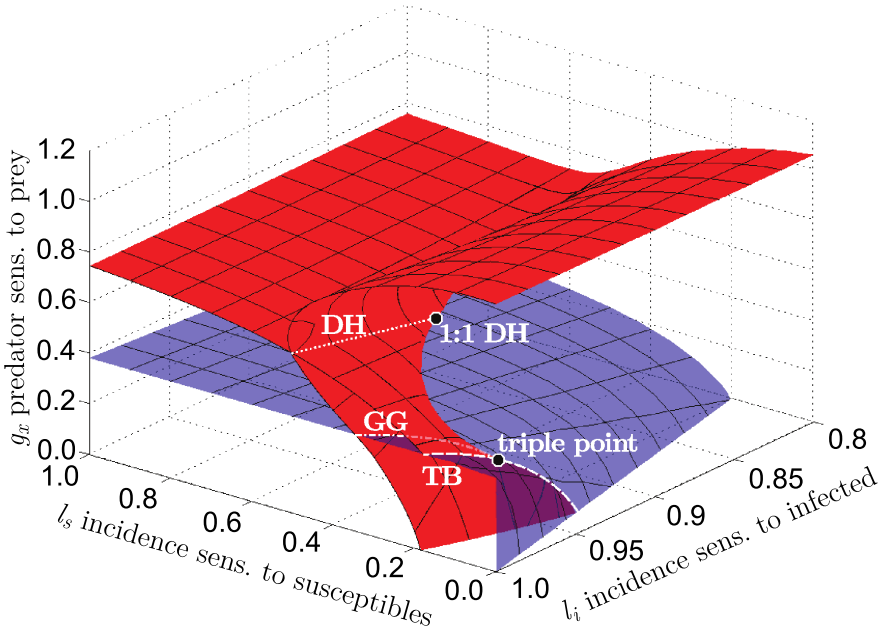

Figure 2: Re-printed with permission from [50]; see also [53]. The red surface indicates Hopf bifurcation and the blue surface saddle-node bifurcations. Higher co-dimension bifurcations are indicated by separate labels. The main codimension two curves are Gavrilov-Guckenheimer (GG), Takens-Bogdanov (TB) and double-Hopf (DH) bifurcations.

Figure 2 shows a good example what type of information we can obtain focusing on the elasticities; the scale parameters have been fixed to biologically reasonable values [50]. The three-dimensional bifurcation diagram shows codimension one bifurcation surfaces (fold and Hopf) as well as codimension two curves (Gavrilov-Guckenheimer, Takens-Bogdanov and

double-Hopf) and codimension three points (1 : 1 resonance, triple point [41, 14]). Although not all the unfoldings of the higher-codimension bifurcations are known it often suffices to detect the bifurcation point as an organizing center to gain insight into the overall dynamics. For example, parts of the double-Hopf bifurcation are known to generate chaotic dynamics due to associated torus and homoclinic bifurcations [24]. Although we cannot conclude chaotic dynamics for the scale parameters chosen in Figure 2 we can conclude that varying a sufficiently large number of them we expect chaotic dynamics to occur generically for many specific models derived from (52).

6.3 Food Webs

The underlying question addressed in [22] is what factors stabilize a food web. The model considers the evolution of N population densities X_i given as

$$X_i' = S_i(X_i) + F_i(X_1, \ldots, X_N) - M_i(X_i) - \sum_{j=1}^{N} G_{ij}(X_1, \ldots, X_N) \tag{54}$$

where S_i is the gain due to primary production, F_i is the gain due to predation, M_i is the loss due to natural mortality and G_{ij} is the loss due to predation. The equations (54) are a natural candidate to apply generalized modeling since one might have some information about the unknown functional forms but it might be too restrictive to just consider a single specific model. For the definitions and interpretations of the generalized parameters we refer to [22]. The interactions between the different specifies are described by the coupling terms F_i and G_{ij}. Now one can analyze the stability of food webs with the following basic steps:

(1) Consider a set of generalized parameters.

(2) Sample one food web (i.e. the predator-prey interaction links and their strength).

(3) Check whether the equilibrium point $x = 1$ is stable.

To draw conclusions from this approach the steps (2)-(3) were repeated for 10^8 food webs for a fixed number of species. The network was assumed to consist of one connected component and contains no double links or loops. The correlation of a parameter p with stability was defined by

$$R := \frac{\sum_{l=1} \nu_s p_{s,l} - \frac{\nu_s}{\nu} \sum_{l=1}^{\nu} p_l}{\nu \sigma_p \sigma_s}$$

where $p_{s,l}$ is the sets of parameters giving rise to stable webs, p_l is the entire set of parameter values considered, ν is the number of elements in $\{p_l\}$, ν_s is the number of elements in $\{p_{s,l}\}$, σ_p is the standard deviation of p and σ_s is the standard deviation of the stability with $s_l = 1$ for a stable web and $s_l = 0$ for an unstable one. The value of R and the interpretations of the generalized parameters can then be used to conclude what properties promote or diminish food web stability i.e. which properties are positively or negatively correlated to stability. In addition, the topology of the food web has been investigated by varying the number of species N; for example, the relation between the number of links L and the number of species has been considered. The main results are:

- Higher variability in link strength stabilizes small food webs but destabilizes large ones.
- Stability scales as a power law with the number of species and their connectance.
- Stability is enhanced by high trophic level species feeding on multiple prey species and also by intermediate level species being fed upon by multiple predators.

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