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Reliable computation of equilibrium states and bifurcations in ecological systems analysis

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Abstract

A problem of frequent interest in analyzing nonlinear ODE models of ecological systems is the location of equilibrium states and bifurcations. Interval-Newton techniques are explored for identifying, with certainty, all equilibrium states and all codimension-one and codimension-two bifurcations of interest within specified model parameter intervals. The methodology is applied to a tritrophic food chain in a chemostat (Canale's model), and a modification of thereof. This modification aids in elucidating the nonlinear effects of introducing a hypothetical contaminant into a food chain.

Keywords: Ecosystem modeling; Ecological risk assessment; Food chains; Equilibrium states; Bifurcations; Nonlinear dynamics

1. Introduction

Ecological systems, including food chains and food webs, are often modeled using systems of nonlinear ordinary differential equations (ODEs). Of particular interest here is the modeling of food chains, which provides challenges in the fields of both theoretical ecology and applied mathematics. Food chain models are descriptive of a wide range of behaviors in the environment, and are useful as a tool to perform ecological risk assessments (Naito, Miyamoto, Nakanishi, Masunaga, & Bartell, 2002). These models are often simple, but display rich mathematical behavior, with varying numbers and stability of equilibria and limit cycles that depend on the model parameters (e.g., Gragnani, De Feo, & Rinaldi, 1998; Moghadas & Gumel, 2003). Many different model formulations are possible, depending on the number of species analyzed, the predation responses used, whether age or fertility structure is of interest for a given species, and how resources are being modeled for the basal species. Analysis of food chain models is often performed by examining the parameter space of the model in one or more variables. This approach is referred to as bifurcation analysis, and it provides a powerful tool for concisely representing a large amount of information regarding both the number and stability of equilibrium states (steady states) in a model. In a two-parameter bifurcation diagram, the shape of bifurcation curves can elucidate the dependence, or lack there of, between model parameters, which in turn can provide information on their ecological relevance. Furthermore, both the shape and the order of bifurcation curves in a diagram can be used to make comparisons between different food chain models. We will focus on one particular food chain model here, namely Canale's chemostat model, as described in detail below. We will also develop and study a version of the model that incorporates an ecosystem contaminant.

Determining the equilibrium states and bifurcations of equilibria in a nonlinear dynamical system is often a challenging problem, and great effort can be expended in analyzing even a relatively simple food chain model with nonlinear functional responses. For simple systems, or specific parts of more complex ones, analytic techniques and isocline analysis may be useful. However, for more complex problems, numerical continuation methods are the predominant computational tools, with packages such as AUTO (Doedel et al., 2002), MATCONT (Dhooge, Govaerts, & Kuznetsov, 2003) and others being particularly popular in this context. Continuation methods can be quite reliable, especially in the hands of an experienced user. However, in general, continuation methods are initialization dependent and provide no guarantee that all equilibrium states and all bifurcations of equilibria will be found. Thus, effective use of continuation methods may require some *a priori* understanding of system behavior in order to reliably create an accurate bifur-

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cation diagram. Gwaltney, Styczynski, and Stadtherr (2004) described an alternative approach, based on interval mathematics, and applied it to a simple tritrophic Rosenzweig–MacArthur model, and variations thereof. We will explore the use of the same approach here, but apply it to more complex models. This computational method uses an interval-Newton approach combined with generalized bisection, and provides a *mathematical and computational guarantee* that *all* equilibrium states and bifurcations of equilibria will be located, without need for initializations or *a priori* insights into system behavior. There are other dynamical features of interest in food chain models, such as limit cycles (and their bifurcations); however, our attention here will be limited to equilibrium states and their bifurcations. Interval methodologies have been successfully applied to the problem of locating equilibrium states and singularities in traditional chemical engineering problems, such as reaction and reactive distillation systems. Examples of these applications are given by Schnepper and Stadtherr (1996), Gehrke and Marquardt (1997), Bischof, Lang, Marquardt, and Mönnigmann (2000), and Mönnigmann and Marquardt (2002).

Our interest in ecological modeling is motivated by its use as one tool in studying the impact on the environment of the industrial use of newly discovered materials. Clearly it is preferable to take a proactive, rather than reactive, approach when considering the safety and environmental consequences of using new compounds. Of particular interest is the potential use of room temperature ionic liquid (IL) solvents in place of traditional solvents (Brennecke & Maginn, 2001). IL solvents have no measurable vapor pressure (i.e., they do not evaporate) and thus, from a safety and environmental viewpoint, have several potential advantages relative to the traditional volatile organic compounds (VOCs) used as solvents, including elimination of hazards due to inhalation, explosion and air pollution. However, ILs are, to varying degrees, soluble in water; thus if they are used industrially on a large scale, their entry into the environment via aqueous waste streams is of concern. The effects of trace levels of ILs in the environment are today not well known and thus must be further studied. Ecological modeling provides a means for studying the impact of such perturbations on a localized environment by focusing not just on single-species toxicity information, but rather on the larger impacts on the food chain and ecosystem. Of course, ecological modeling is just one part of a much larger suite of tools, including toxicological (e.g., Bernot, Brueseke, Evans-White, & Lamberti, 2005; Bernot, Kennedy, & Lamberti, 2005; Ranke et al., 2004; Stepnowski, Skladanowski, Ludwiczak, & Laczynska, 2004), microbiological (e.g., Docherty & Kulpa, 2005; Pernak, Sobaszkiewicz, & Mirska, 2003) and other (e.g., Gorman-Lewis & Fein, 2004; Ropel, Belvèze, Aki, Stadtherr, & Brennecke, 2005) studies, that must be used in addressing this issue.

2. Problem formulation

2.1. Canale's chemostat model

Canale's chemostat model is a tritrophic (prey, predator, superpredator) food chain model embedded in a chemostat (a constant volume system, with constant flow in and out). The predator and superpredator grow by consuming the prey and predator species, respectively, while the prey grows by consuming nutrients in the chemostat. The rate at which the prey, predator, and superpredator consume food is modeled by a hyperbolic functional response. The hyperbolic, or Holling Type II, functional response has become the favored way to model feeding rates in theoretical ecology. This type of response is mathematically more complicated than a simple linear response, but provides a leveling-off (saturation) effect that is a more realistic model of behavior observed in the environment. There is a constant flow through the chemostat, which carries nutrients into the system, and which carries nutrients and organisms out of the system. The model is given by the following balance equations:

$$\frac{dx_0}{dt} = D(x_n - x_0) - \frac{a_1 x_0 x_1}{b_1 + x_0} \tag{1}$$

$$\frac{dx_1}{dt} = x_1 \left[e_1 \frac{a_1 x_0}{b_1 + x_0} - \frac{a_2 x_2}{b_2 + x_1} - d_1 - \varepsilon_1 D \right] \tag{2}$$

$$\frac{dx_2}{dt} = x_2 \left[e_2 \frac{a_2 x_1}{b_2 + x_1} - \frac{a_3 x_3}{b_3 + x_2} - d_2 - \varepsilon_2 D \right] \tag{3}$$

$$\frac{dx_3}{dt} = x_3 \left[e_3 \frac{a_3 x_2}{b_3 + x_2} - d_3 - \varepsilon_3 D \right] \tag{4}$$

Here x_0 is the nutrient concentration in the system and x_1, x_2, and x_3 are the biomasses of the prey, predator, and superpredator populations, respectively. The (nonnegative) parameters a_i, b_i, d_i, and e_i are the maximum predation rate, half-saturation constant, density-dependent death rate, and predation effciency of the prey ($i = 1$), predator ($i = 2$), and superpredator ($i = 3$) species. The parameter x_n is the nutrient concentration flowing into the system, and the parameter D is the inflow, or dilution, rate (equal to the outflow rate). The term $\varepsilon_i D$ is the density-dependent washout rate of species i. The constant $\varepsilon_i \in [0, 1]$ quantifies how well a species is able to resist washout. For instance, if $\varepsilon_i = 1$, the organism will be unable to resist washout. An example of such a species would be a unicellular algae. Conversely, if $\varepsilon_i = 0$, the organism is completely resistant to washout. Positive terms on the right-hand sides of Eqs. (1)–(4) represent inflow of nutrient and organism growth. Negative terms represent outflow and consumption of nutrient, and loss of organisms due to predation, washout, and death. This model has received considerable attention in the field of theoretical ecology (Boer, Kooi, & Kooijman, 1998; El-Sheikh & Mahrouf, 2005; Gragnani et al., 1998; Kooi, 2003; Kooi, Boer, & Kooijman, 1997).

As previously stated, our interest in ecological modeling is motivated by its use as a tool for assessing the risk of the industrial use of newly discovered materials, which may enter the environment as contaminants. Many ecologists recognize that ecosystem modeling is important for estimating risk to ecological systems. However, most current assessment methods rely on examining single-species endpoint tests, such as survival, growth and reproductive rates (Pastorok, 2003). Ecological risk estimation using food web models is becoming a more popular method (Bartell, Gardner, & O'Neill, 1992; Bartell, Lefebvre, Kaminski, Carreau, & Campbell, 1999; Lu, Axe, & Tyson, 2003;