Determining Parameters Leading to Chaotic Dynamics in Systems

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1 Introduction

Although the overall prevalence of chaotic dynamics in biological systems is not entirely understood, it is well known that chaos occurs in many natural biological systems involving population dynamics [**?**, **?**, **?**, **?**]. Becks et al. demonstrated existence of chaotic and non-chaotic states in an experimental study of a microbial system with a nutrient source, a predator species, and two prey species, one of which was less preferred by the prey [**?**]. By measuring the population size of each species on a daily basis, the authors were able to document transitions between chaotic and non-chaotic states after changing the strength of the nutrient source.

Models of population dynamics give us a means of better understanding chaotic dynamics in biological systems, and even simple dynamical system models are known to exhibit chaotic behavior for certain values of system parameters [**?**]. Unfortunately, even simple systems can exhibit a range of chaotic and non-chaotic behavior, related in some non-trivial way to certain combinations of system parameters and initial conditions. In this work, we

describe a computational framework that can help researchers develop a better understanding of the causes of chaotic behavior in dynamical systems. These tools allow for efficient systematic exploration of the parameter space of the system to allow characterization and visualization of factors leading to chaotic behavior.

We consider models of bacterial populations which incorporate both predator and prey species, along with a nutrient source. These systems have been well-studied in chemostat environments, both experimentally [**?**, **?**] and analytically [**?**]. They have been shown to demonstrate chaotic dynamics [**?**, **?**] and can be considered as small-scale studies for larger ecological systems [**?**].

In general, we consider the set of coupled differential equations

$$\begin{aligned} \frac{dY_1}{dt} &= f_1\left(Y_1, \ldots, Y_n\right) \\ &\vdots \\ \frac{dY_n}{dt} &= f_n\left(Y_1, \ldots, Y_n\right) \end{aligned}$$

where $Y_1 \ldots Y_{n-1}$ represent population levels of various predator or prey species and Y_n represents the abundance of a nutrient source. The functions on the right-hand side are determined using principles of mass balance, mass action, and enzyme kinetics. The standard approach uses growth rates that are enzyme mediated [**?**], which means the rates are defined as limiting functions which caps the ability of the bacterial populations to grow based on defined saturation-limited values. These principles are rooted in Michaelis-Menten kinetics [**?**, **?**] and are part of the standard approaches used to model systems in a chemostat or other bacterial environments (see, for instance, [**?**, **?**, **?**, **?**, **?**, **?**, **?**] and references therein).

Given the wide applicability of these models to different physical and ecological systems, we seek to better understand the choices of model parameters and initial conditions leading to chaotic behavior. Let $P \subseteq \mathbf{R}^m$ denote all possible valid settings for the m parameters in our system (e.g., one parameter might describe the dilution rate – the rate at which nutrient is introduced into the system). Let $I \subseteq \mathbf{R}^n$ denote the set of all valid initial conditions for $(Y_1, Y_2, \ldots, Y_n)$. Defining $S = P \times I$, we seek to characterize the regions of S leading to chaotic behavior. A particular $s \in S$ is deemed chaotic if it yields a positive Lyapunov exponent, using standard numerical integrators for ordinary differential equations along with popular methods for numerical Lyapunov exponent calculation [**?**, **?**].

Let $C \subseteq S$ denote the subset of all parameters and initial conditions leading to chaotic behavior (a positive Lyapunov exponent). The main result of this paper is a software platform to help researchers characterize the structure of C for any dynamical system – a challenging task due to its high-dimensional nature. The two main components in our system are (1) a method for efficiently generating a representative set of values from C using successive applications of Metropolis-Hastings sampling to a "smoothed out" Lyapunov exponent landscape, and (2) interactive exploratory visualization of the results on a parallel coordinate system. This method of visualization allows the user to observe correlations among pairs of parameters leading to chaotic behavior, and also to conduct exploratory testing for specific "what if" scenarios – for example investigating whether chaotic behavior can be obtained even for highly-restricted ranges of certain parameters.

The remainder of this paper is organized as follows. In Section **??**, we describe the algorithms and visualizations used in our framework. In Section 2, we then describe the results of our framework applied to three models for microbial populations. Finally, we summarize our findings and provide discussion on future research directions in Section 3.

2 Numerical Results

We tested the ability of our algorithm to find parameter settings leading to chaotic states using three example problems, which we describe in this section. We begin the system presented by Kot, et.al., [**?**], where the authors

The ability of our algorithm was

There are three results to report:

- Results from Kot paper which verify the algorithm works
- Results from "Becks" system varying the dilution rate keeping other parameters constant that verify what they observed experimentally
- Results from "Becks" system where several parameters are varied and multiple chaotic states are realized
- Do we want to include computational timings for example problems? Perhaps provide timing for computing Lyapunov exponent, followed by discussion of number of times this procedure is called.

2.1 Kot Equations

We evaluate our framework using the dynamical systems presented and analyzed in work by Kot, Sayler, and Schultz [**?**]. The authors of that work analyze a forced double-Monod model in an initial effort to understand chaos in biological systems. While experimental results are not included in the paper, the authors justify their choice to study this particular system by noting the possibility of obtaining experimental validation of their work. As our primary interest in developing the framework presented here is to aid biologists in their data-based studies of dynamical systems, this particular problem presents an ideal benchmark case.

The dimensionalized equations are given as [**?**]

$$\begin{aligned}
\frac{dS}{dt} &= D\left[S_i\left(1+\epsilon\sin\left(\frac{2\pi}{T}t\right)\right)-S\right]-\frac{\mu_1}{Y_1}\frac{SH}{K_1+S}\\
\frac{dH}{dt} &= \mu_1\frac{SH}{K_1+S}-DH-\frac{\mu_2}{Y_2}\frac{HP}{K_2+H}\\
\frac{dP}{dt} &= \mu_2\frac{HP}{K_2+H}-DP
\end{aligned}$$

where S represents the limiting substrate, H represents a prey species, and P represents a predator species. We note the predator species consumes only the prey, so its population is indirectly associated with the changes in S. The parameters in the model govern the response of the organisms to changes in the system. D is the dilution rate, which defines the ratio of the flow into the chemostats to the volume of organisms in the chemostat; μ_1 and μ_2 are the maximum specific growth rates of the prey and predator, respectively; Y_1 is the yield of prey per unit mass of substrate, and Y_2 is the yield of predator per unit mass of prey; and K_1 and K_2 are the half-saturation constants [**?**]. S_i is the inflowing substrate concentration [**?**].

The equations are non-dimensionalized by rescaling all variables by the inflow substrate, the prey by its yield constant Y_1, and the predator by both yield constants [**?**]. The dimensionless system is given by

$$\frac{dx}{d\tau} = 1+\epsilon\sin(\omega\tau)-x-\frac{Axy}{a+x} \tag{1}$$

$$\frac{dy}{d\tau} = \frac{Axy}{a+x}-y-\frac{Byz}{b+y} \tag{2}$$

$$\frac{dz}{d\tau} = \frac{Byz}{b+y}-z, \tag{3}$$

where $x = \dfrac{S}{S_i}$, $y = \dfrac{H}{Y_1 S_i}$, and $z = \dfrac{P}{Y_1 Y_2 S_i}$, $\tau = Dt$, and $\omega = \dfrac{2\pi}{DT}$. Also, $A = \dfrac{\mu_1}{D}$, $a = \dfrac{K_1}{S_i}$, $B = \dfrac{\mu_2}{D}$, and $b = \dfrac{K_2}{Y_1 S_i}$.

The dimensionless system exhibits chaotic behavior for value of $\omega = \dfrac{5\pi}{6}$ and $\epsilon = 0.6$ [**?**] using $S_i = 115$ mg/l, $D = 0.1$ / h, and the values of the parameters in Table 1.

	Y_i	μ_i h^{-1}	K_i mg/l
Prey ($i = 1$)	0.4	0.5	8
Predator ($i = 2$)	0.6	0.2	9

Table 1: Values of parameters for microbial model presented in Kot, et.al. [**?**]

2.2 Kravchenko Equations

As a second example system, we consider the models for plant growth promoting rhizobacteria (PGPR) inoculation developed by Kravchenko, Strigul, and Shvytov [**?**] and Strigul and Kravchenko [**?**]. The model equations studied in that work are

$$\frac{dX}{dt} = X\left(\mu_X\left[S, P, N\right] + F\left[Z\right] - \alpha X - d_1\right) \tag{4}$$

$$\frac{dZ}{dt} = Z\left(\mu_z\left[S, P, N\right] + G\left[X\right] - \beta Z - d_2\right) \tag{5}$$

$$\frac{dS}{dt} = W\left(t\right) + L - D_S\left(S - S_0\right) - \frac{X\mu_x\left[S, P, N\right]}{Y_{XS}} - \frac{Z\mu_z\left[S, P, N\right]}{Y_{ZS}} \tag{6}$$

$$\frac{dP}{dt} = D_P\left(P_0 - P\right) - \frac{X\mu_x\left[S, P, N\right]}{Y_{XP}} - \frac{Z\mu_z\left[S, P, N\right]}{Y_{ZP}} \tag{7}$$

where X and Z represent the concentration of PGPR and resident microorganisms, respectively, S represents an organic substrate concentration, and P represents the concentration of oxygen in the soil [**?**]. The parameters μ_X and μ_Z are growth rates dependent on the available substrate S, oxygen P, and nitrogen N through defined growth rate functions. These functions are

rate limited and have the general form [**?**]

$$\mu_* [S, P, N] = \mu_{m*} \frac{S}{S + \theta K_{S*}} \frac{P}{P + K_{P*}} \frac{N}{N + \theta K_{N*}},$$

where μ_{m*} is a specified maximal growth rate for the species of interest, θ is the moisture content of the soil, and K_{S*} represents an affinity constant for the species to the organic substrate. The constants K_{N*} and K_{P*} are similarly defined. It is easily seen they have the general form associated with general rate limited models of interest in this work. The initial values of the parameters used in our work are provided in detail in the paper by Strigul and Kravchenko [**?**].

The function $W(t)$ is meant to simulate the effects of photosynthesis, and is therefore periodic with period length 24 h. We incorporate this into our model system using a Fourier series expansion of the piecewise constant function

$$f(x) = \begin{cases} 1, & 0 < x \leq 12 \\ 0, & 12 < x < 24 \end{cases}$$

2.3 Becks Equations

For the third example, we attempt to model a set of experimental data where chaotic states were demonstrated for varying levels of the dilution parameter [**?**]. The authors of that work describe experimental scenarios where the system under study could transition from chaotic to equilibrium states, and vice versa, by crossing a threshold value for the dilution rate.

We describe the data using a set of rate-limited, dynamical equations similar to the previous examples. The general description of the system we consider is given by

$$\frac{dR}{dt} = R\left[\mu_{NR}\left(\frac{N}{K_{NR} + N}\right) - \delta_R\right] - \frac{\mu_{PR}}{Y_{PR}}\left(\frac{R}{K_{PR} + R}\right) P - DR \tag{8}$$

$$\frac{dC}{dt} = C\left[\mu_{NC}\left(\frac{N}{K_{NC} + N}\right) - \delta_C\right] - \frac{\mu_{PC}}{Y_{PC}}\left(\frac{C}{K_{PC} + C}\right) P - DC \tag{9}$$

$$\frac{dP}{dt} = P\left[\mu_{PR}\left(\frac{R}{K_{PR} + R}\right) + \mu_{PC}\left(\frac{C}{K_{PC} + C}\right) - \delta_P\right] - DP \tag{10}$$

$$\frac{dN}{dt} = DN_0 - R\left[\frac{\mu_{NR}}{Y_{NR}}\left(\frac{N}{K_{NR} + N}\right)\right] - C\left[\frac{\mu_{NC}}{Y_{NC}}\left(\frac{N}{K_{NC} + N}\right)\right] - DN. \tag{11}$$

The variables R and C represent the prey species of rods and cocci, respectively. We let P represent the predator species, and N represents a nutrient source to the system. The parameter D represents dilution rate for input of nutrients to the system.

The parameters in the model determine the feeding habits of the predator and prey, as well as death and growth rates for each species. These parameters may be used to specify particular behaviors of the organisms, e.g., growth rates due to feeding on nutrient sources rather than prey. We define μ_{N*} as maximum growth rates for the associated species based on consumption of nutrients and μ_{P*} as the maximum growth rates for predator based on consumption of the associated prey species. The value of K_{N*} is the half saturation constant for the species on the nutrient, and K_{P*} is the half saturation constant for the predator on the associated species. Note these latter constants may determine a "preference" for one prey over the other. The parameters Y_{N*} denote represent yield coefficients for the species on the nutrient, while Y_{P*} denote the yield coefficients for the predator associated with the prey species.

Death rates for each species are given by δ_*

The model equations and system parameters were estimated by Molz as part of his earlier work [**?**]. The intent was to derive a mathematical model whose dynamics closely resembled the experimental dynamics seen in Becks, et.al. [**?**]. We begin with initial populations for the

Specific values of the parameters used for the model are provide in Table 2.

	Species		
Parameter	R	C	P
μ_{N*}	12 / day	6 / day	
μ_{P*}	2.2 / day	2.2 / day	
K_{N*}	8e-6 gm/cc	8e-6 gm/cc	
K_{P*}	1e-6 gm/cc	1e-6 gm/cc	
Y_{N*}	0.1 gm R / gm N	0.1 gm C / gm N	
Y_{P*}	0.12 gm P / gm R	0.12 gm P / gm C	
δ_*	0.5 / day	0.25 / day	0.08 / day

Table 2: Table of values for model equations (8) - (11) used in the numerical simulations.

We note the model involves altogether fifteen parameters. The parameter space can be reduced by rescaling the state variables R, C, P and N, and time T. Rescaling the equations eliminates four of the parameters and simultaneously makes the system more perspicuous for both qualitative analysis and numerical simulation. The rescaling is not unique and can be used for different purposes. For this third example problem, we introduce the following change of variables,

$$R = K_{PR}\, r, \quad C = K_{PC}\, c, \quad P = \frac{K_{PR} Y_{PR}\,(\delta_R + D)}{\mu_{PR}}\, p, \tag{12}$$

$$N = K_{NR}\, n, \quad T = \frac{1}{\delta_R + D}\, t, \tag{13}$$

where the lowercase r, c, p, n and t are the new rescaled variables and time, respectively. The rescaled model equations are given by

$$\frac{dr}{dt} = \widehat{\mu}_{NR}\left(\frac{nr}{n+1}\right) - \left(\frac{rp}{r+1}\right) - r \tag{14}$$

$$\frac{dc}{dt} = \widehat{\mu}_{NC}\left(\frac{nc}{n+\widehat{\kappa}}\right) - \widehat{\eta}_1\left(\frac{cp}{c+1}\right) - \widehat{\delta}_C\, c \tag{15}$$

$$\frac{dp}{dt} = \widehat{\mu}_{PR}\left(\frac{rp}{r+1}\right) + \widehat{\mu}_{PC}\left(\frac{cp}{c+1}\right) - \widehat{\delta}_P\, p \tag{16}$$

$$\frac{dn}{dt} = \widehat{\delta}\,(n_0 - n) - \widehat{\eta}_2\left(\frac{nr}{n+1}\right) - \widehat{\eta}_3\left(\frac{nc}{n+\widehat{\kappa}}\right), \tag{17}$$

where the new (eleven) parameters are expressed in terms of the original parameters as follows:

$$\widehat{\mu}_{NR} = \frac{\mu_{NR}}{(\delta_R + D)}, \quad \widehat{\mu}_{NC} = \frac{\mu_{NC}}{(\delta_R + D)}, \tag{18}$$

$$\widehat{\mu}_{PR} = \frac{\mu_{PR}}{(\delta_R + D)}, \quad \widehat{\mu}_{PC} = \frac{\mu_{PC}}{(\delta_R + D)}, \tag{19}$$

$$\widehat{\kappa} = \frac{K_{NC}}{K_{NR}}, \; \widehat{\delta}_C = \frac{\delta_C + D}{(\delta_R + D)}, \; \widehat{\delta}_P = \frac{\delta_P + D}{(\delta_R + D)}, \; \widehat{\delta} = \frac{D}{(\delta_R + D)}, \tag{20}$$

$$\widehat{\eta}_1 = \frac{\mu_{PC} Y_{PR} K_{PR}}{\mu_{PR} Y_{PC} K_{PC}}, \; \widehat{\eta}_2 = \frac{\mu_{NR} K_{PR}}{Y_{NR} K_{NR}\,(\delta_R + D)}, \; \widehat{\eta}_3 = \frac{\mu_{NC} K_{PC}}{Y_{NC} K_{NR}\,(\delta_R + D)}. \tag{21}$$

We also introduce the initial value for the rescaled nutrient source, $n_0 = K_{NR} N_0$.

3 Conclusions

We have provided a framework that allows researchers to efficiently search over a design space including parameter values and initial conditions and discover possible connections between values of these constants and chaotic dynamics. It is possible that the ability for such a search will reveal chaotic behavior in systems not previously know to have chaotic regime and reveal the existence of parameters and initial conditions not previously known to yield chaotic behavior in known systems.

- Outline ability to understand dynamics for wide variety of parameter changes
- Emphasize this is easily handled computationally but virtually impossible in a laboratory environment
- One objective is to provide a tool for those wishing to analyze systems for chaotic dynamics without the need for rigorous mathematical analysis
- We have verified what is in the literature
- The environment is embarrassingly parallelizable; thus, significant speedups can be realized.

4 Possible journals

1. J. of Biological system
2. J. of Bioinformatics and Computational biology
3. J. of computer science and systems biology
4. PLoS Computational Biology
5. http://biosystems.ucsf.edu/journals.html
6. Communications in Nonlinear Science and Numerical Simulation

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