NIMBioS SRE guide 2020

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This document gives a basic set of guidelines to begin fitting dynamic models to laboratory growth data. I will add to this document as we progress through June. The guidelines are separated into two sections. The first section centers around mathematical modeling, and gives a worksheet style intro to numerical integration. The second section centers more around data manipulation. The third section describes how to pull together the model and the data.

It is up to you, the students, to decide how to approach different sections. You can either tackle both sections together, or divide and conquer.

1   Modeling

The goal of the following is to build understanding of numerical integration in a step-wise manner. We begin with a trivial example, and go on to layer in more complex examples.

1.1   Trivial example

Begin with the simple model:

$$\frac{dP}{dt} = \mu P \tag{1}$$

Subject to the initial condition $P(0) = P_0$. Here, P is a phytoplankton cell density (cells ml^{-1}), and P_0 is an arbitrary starting concentration. The parameter μ is a phytoplankton growth rate with units day^{-1}. Typically, growth rates are in the range 0-3.

You can solve this model algebraically by separation of variables. You can also approximate the true solution using numerical integration. Many alternatives for numerical integration exist. I recommend starting with the simplest, Euler integration.

I recommend that you find the closed form solution, plot it, and compare the numerical approximation. You can do this in any programming language, but Python's numpy package may be a good choice for our purposes.

Once you have some operational code, test to see how altering your step-size changes the quality of the approximation

1.2 The odeint package

Euler integration is the simplest choice for numerical integration, and it is often highly inefficient and numericall inaccurate. Python's odeint package includes Euler integration, along with many more sophisticated integration algorithms. I recommend using the odeint package to numerically solve the above model. Compare your odeint solution against the closed form solution, and the Euler approximation from section 1.1.

1.3 A simple virus infection model

We can now move on to a slightly more complex example. Consider the coupled model:

$$\frac{dP}{dt} = \mu P - \phi V P \tag{2}$$

$$\frac{dV}{dt} = \beta \phi V P - \delta V \tag{3}$$

where P is again a phytoplankton cell density, and V is now a virus particle density (units ml^{-1}). The parameter ϕ is a virus affinity for phytoplankton cells, with units (ml time^{-1}. The parameter δ is a virus decay rate with units time^{-1}. You can choose arbitrary initial conditions for this system of equations, e.g. P_0 and V_0.

I am not aware of a closed form solution to this model. Can you use Euler integration and / or the odeint package to approximate the solution to this model? For now, you can choose arbitrary values for each parameter to get qualitatitively plausible solutions.

1.4 Model with one infected class

Now let's consider a model with an infected state, I:

$$\frac{dP}{dt} = \mu P - \phi V P \tag{4}$$

$$\frac{dI}{dt} = \phi V P - \lambda I \tag{5}$$

$$\frac{dV}{dt} = \beta \lambda I - \delta V \tag{6}$$

Now λ is a rate of lysis. Can you approximate the solution to this model for an arbitrary choice of λ and with $I(0) = 0$?

2 Data manipulation

Let's start by loading data into Python and visualizing it. In the github repository, find the data files: 'Baudoux32_PGV01T_Control.txt', 'Baudoux32_PGV01T_Infected.txt', and 'Baudoux32_PGV01T_Virus.txt'. Respectively, these data are virus-free controls

(as in Eq 1); cell densities during infection (effectively, this is P in Eqs 2, or $P+I$ in Eqs 4-5); and virus densities during infection (V in Eq. 3 or 6).

In each file the left-most column is a time, in days, and the right-most column is the datapoint corresponding to each state-variable. Start by loading these files into Python and plotting them. I will leave it to you to determine the optimal way to do this.

3   Model-data comparison

In the github repository, there is a file in the figures directory called 'ModelTester.pdf'. The first page here shows a couple of example of models (solid lines) compared with the Baudoux32 data. These are model fits to the data. Can you take the models from section 1 and compare them with the data loaded in section 2? Feel free to use trial and error to find parameter values which allow the best match of model solutions with data. Note that, the 'ModelTester.pdf' file does not include data for the 'controls' (virus-free growth curves). It might actually be easiest if you start by comparing the solution to Eq 1 with the 'Baudoux32_PGV01T_Control.txt' data, and adding in the infection experimental data and models with V state-variables later.