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Ordinary Differential Equations, Oscillating Chemical Reactions, and Chaos

Chaos has been found in many aspects of the phsyical world ranging from the weather to the human heartbeat [1]. Some concrete and definable examples of chaos can be seen in oscillating chemical reactions.

One example is the Belousov-Zhabotinskii reaction in chemistry. By changing the rate at which reactants are fed into the system, the oscillations can change from periodic behavior to chaotic.

The chemistry of the BZ reaction is rather complex, and involves the oxidation of easily brominated organic material by bromate ion in an acidic environment, which makes it rather difficult to model ([2],[3],[4]).

Slightly simpler is a similar reaction involving a three-variable autocatalator [5]. Autocalators involve isothermal reactions of chemicals in a thermodynamically closed environment – that is, reactions that maintain a constant temperature. Two-variable autocatalators have been successful in reproducing many types of chemical oscillations; a chemical modification by Peng et al. produced a three-variable autocalator which shows complex periodic as well as chaotic behavior. The chemistry of this reaction is as follows:

$$\begin{aligned} P &\longrightarrow A \\ P + C &\longrightarrow A + C \\ A &\longrightarrow B \\ A + 2B &\longrightarrow 3B \\ B &\longrightarrow C \\ C &\longrightarrow D \end{aligned}$$

This chemistry can be modeled by the following differential equations:

$$\frac{dA}{dt} = k_1 P + k_2 PC - k_3 A - k_4 AB^2$$

$$\frac{dB}{dt} = k_3 A + k_4 AB^2 - k_5 B$$

$$\frac{dC}{dt} = k_4 B - k_5 C$$

This can be converted into the following dimensionless form:

$$\frac{dX}{d\tau} = c_1 + c_2 Z - X - XY^2$$

$$c_3 \frac{dY}{d\tau} = X + XY^2 - Y$$

$$c_4 \frac{dZ}{d\tau} = Y - Z$$

In the equations above c_i are constants, and X, Y, and Z are proportional to A, B, and C respectively.

Message to the wise and foolhardy: The "final product" of this assignment is a bifurcation diagram showing the changing behavior of with respect to c2. Jumping in head-first and writing working code that produces impressive bifurcation images in a single session would be a pretty neat trick. The sane experienced programmer, humbled by days of searching for silly mistakes, would follow the baby-steps listed below, since debugging bit-by-bit (excuse the pun) is much easier than troubleshooting the entire program at once. This "baby-steps" methodology is the key to successfully building any program that is made of multiple components[6].

1. Creating a Function to Implement Euler's Method

a.) Use Euler's method to plot:

$$\frac{dy}{dt} = y \qquad y(0) = 1$$

Compare your results to a graph of $y = e^t$. Notice how the size of the time steps and number of iterations affect the accuracy of your results.

b.) Use Euler's method to plot:

$$\frac{dy}{dt} = k \times cos(t) \qquad y(0) = 0 \qquad k = 1$$

Compare your results to a graph of $y = sin(t)$. Again notice the effect of varying the time step size and number of iterations.

Save a copy of this code for use in 3a.

2. Finding peaks

The y-values plotted in the bifurcation diagram ar eactually the peak y-values shown against their respective c_2-values, which makes this step an integral one.

a.) Devise an algorithm to locate the peaks of:

$$\frac{dy}{dt} = k \times cos(t) \qquad y(0) = 0 \qquad k = 1$$

b.) Modify the algorithm so that each peak value is returned only once. Insure that it will still return all of the peaks of multiple peak functions like:

$$\frac{dy}{dt} = cos(t) + 2sin(t) \qquad y(0) = 0$$

By stopping the same peaks from redundantly being returned, this step serves as an important time saver.

c.) Varying k from 1 to 5, plot the peaks of:

$$\frac{dy}{dt} = k \times cost(t) \qquad y(0) = 0$$

against the changing values of k. You should have a straight line stretching from (1,1) to (5,5).

3. Solving for a system of Oscillating Differential Equations

a.) Using the code from step 1 and the three autocatalator equations, plot $log(y)$ against time. Use the following values for the constants:

$$c_1 = 10 \qquad c_2 = 0.15 \qquad c_3 = 0.005 \qquad c_4 = 0.02$$

You should have an oscillating graph.

b.) Using the code from step 2c and the three equations, vary c_2 from 0.10 to 0.18 with very small intervals (0.0005 or less), and plot the peaks y against their respective values of c2. This should yield a birfurcation diagram.

4. Implementing the Fourth-Order Runge-Kutta Method

a.) Use Runge-Kutta to plot:

$$\frac{dy}{dt} = y \qquad y(0) = 1$$

and

$$\frac{dy}{dt} = k \times cos(t) \qquad y(0) = 0 \qquad k = 1$$

Compare your results to graphs of $y = sin(t)$ and $y = e^t$ and those created with Euler's method.

b.) Using the code from the previous step and the three autocatalator equations, plot log(y) against time. Use the following values for the constants:

$$c_1 = 10 \qquad c_2 = 0.15 \qquad c_3 = 0.005 \qquad c_4 = 0.02$$

Compare your results with those generated by Euler's Method in 3a.

c.) Combine the Runge-Kutta method with your peak-finding algorithm from step 2 to generate a bifurcation diagram similar to that of step 3b. Compare the graphs. What differences do you find?

5. Constructing the Attractor A strange attractor is essentially a graphical representation of x, y, and z, parametrized by time. It is called an attractor because x, y, and z never stray far from a certain point or points in space. It is considered "strange" because the x, y, and z may infinitely loop around these points of attraction, yet never repeat itself. Thus if one were to follow a line connecting each point to the next, one would find a line of infinite length within the finite volume of the attractor. Consult the Ivview tutorial and then construct an Ivview file that will plot the attractor for $c_2 = 0.153$. Keep the Ivview file size under 1 MB by sampling points on the attractor rather than plotting every point.

EXTRA CREDIT: In a famous paper entitled "Period Three Implies Chaos", mathematician James Yorke proved that in any one-dimensional system in which existed an oscillating state of three values there also exists chaos. A period of three also implies a period of five, though the reverse is not true. Adapt your algorithm so that it finds the period of each oscillating graph (the period of a graph is the number of equilibrium peaks it has before repeating). Determine whether period three and/or period five oscillations are found, and where. What does this imply about the system? Is there really chaos in the system? Explain.

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