

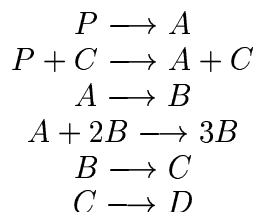
Ordinary Differential Equations, Oscillating Chemical Reactions, and Chaos

Chaos has been found in many aspects of the physical 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]. Autocatalators 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 autocatalator which shows complex periodic as well as chaotic behavior. The chemistry of this reaction is as follows:



This chemistry can be modeled by the following differential equations:

$$\begin{aligned} \frac{dA}{dt} &= k_1P + k_2PC - k_3A - k_4AB^2 \\ \frac{dB}{dt} &= k_3A + k_4AB^2 - k_5B \\ \frac{dC}{dt} &= k_4B - k_5C \end{aligned}$$

This can be converted into the following dimensionless form:

$$\begin{aligned} \frac{dX}{d\tau} &= c_1 + c_2Z - X - XY^2 \\ c_3 \frac{dY}{d\tau} &= X + XY^2 - Y \\ c_4 \frac{dZ}{d\tau} &= Y - Z \end{aligned}$$

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 c_2 . 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:

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

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:

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

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 are actually 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:

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

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:

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

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:

$$\frac{dy}{dt} = k \cos(t) \quad y(0) = 0$$

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:

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

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 c_2 . This should yield a bifurcation diagram.

4. Implementing the Fourth-Order Runge-Kutta Method

a.) Use Runge-Kutta to plot:

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

and

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

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:

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

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. Find a plotting tool that can generate a three-dimensional plot, and use it to plot the attractor for $c_2 = 0.153$. (See the precept on plotting.) To keep the size of the data files manageable (under 1 MB, say), you may want to sample the attractor rather than keeping 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.

References

- [1] J. Gleick. *Chaos*. Viking Penguin, New York, 1987.
- [2] G. L. Baker and J. P. Gollub. *Chaotic Dynamics — An Introduction*. Cambridge University Press, Cambridge, England, 1990.
- [3] G. Rowland. *Non-linear Phenomena in Science and Engineering*. Ellis Horwood, Chichester, England, 1990.
- [4] R. Kapral and K. Showalter. *Chemical Waves and Patterns*. Kluwer Academic Press, Dordrecht, the Netherlands, 1995.
- [5] B. Peng, S. K. Scott, and K. Showalter. Period doubling and chaos in a three-variable autocatalator. *Journal of Physical Chemistry*, 94:5243–5246, 1990.
- [6] F. Oz, (director). *What About Bob?*, 1991. (film), starring Bill Murray and Richard Dreyfuss.
- [7] E. N. Lorenz. Deterministic nonperiodic flow. *Journal of the Atmospheric Sciences*, 20(1):130–141, March 1963.
- [8] S. Krasner. *The Ubiquity of Chaos*. American Association for the Advancement of Science, Washington, D.C., 1990.
- [9] R. J. Field and M. Burger. *Oscillations and Traveling Waves in Chemical Systems*. John Wiley, New York, 1985.
- [10] S. H. Strogatz. *Nonlinear Dynamics and Chaos*. Addison Wesley, Reading, MA, 1994.
- [11] * H. Gould and J. Tobochnik. *An Introduction to Computer Simulation Methods*. Addison Wesley, Menlo Park, Ca., second edition, 1996.
- [12] P. W. Davis. *Differential Equations for Mathematics, Science, and Engineering*. Prentice-Hall, Englewood Cliffs, N.J., 1992.
- [13] W. E. Boyce and R. C. DiPrima. *Elementary Differential Equations*. John Wiley, New York, fifth edition, 1986.