Modeling Notes

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1 Introduction

Mathematical modeling is the process by which we try to convert physical processes into a mathematical context. In so doing, we need to keep some things in mind:

- What assumptions about the physical process are *necessary* in order to emulate the behavior that we observe? In this, we strip away all the irrelevant information so that we can study the behavior in a mathematically ideal context. The assumptions one makes, and how one expresses those assumptions mathematically are the most important step in the modeling process.
- The model should be simple enough so that we can understand it. If a model is so complicated as to defy understanding, then the model is not useful.
- The model should be complex enough so that we capture the desired behavior. The model should not be so simple that it does not explain anything- again, such a model is not useful. This does not mean that we need a lot of equations, however. One of the lessons of *chaos theory*[1] is the following:

  Very simple models can create very complex behavior

- To put the previous two items into context, when we build a model, we probably have some questions in mind that we'd like to answer. You can evaluate your model by seeing if it gives you the answer- For example,
  - Should a stock be bought or sold?
  - Is the earth becoming warmer?
  - Does creating a law have a positive or negative social effect?
  - What is the most valuable property in monopoly?

[1]For a general introduction to Chaos Theory, consider reading "Chaos", by James Gleick. For a mathematical introduction, see "An Introduction to Chaotic Dynamics", by Robert Devaney

In this way, a model provides *added value*, and it is by this property that we might evaluate the goodness of a model.

- Once a model has been built, it needs to be checked against reality- Modeling is not a thought experiment! Of course, you would then go back to your assumptions, and revise, create new experiments, and check again.

You might notice that we have used very subjective terms in our definition of "modeling"- and these are an intrinsic part of the process. Some of the most beautiful and insightful models are those that are elegant in their simplicity. Most everyone knows the following model, which relates energy to mass and the speed of light:

$$E = mc^2$$

While it is simple, the model is also far-reaching in its implications (we will not go into those here). Other models of observed behavior from physics are so fundamental, we even call them physical "laws"- such as Newton's Laws of Motion.

In building mathematical models, you are allowed and encouraged to be creative. Explore and question your assumptions, explore your options for expressing those options mathematically, and most importantly, use your mathematical background.

2 What Kinds of Models Are There?

There are many ways of classifying mathematical models, which will make sense once you begin to build your own models. In general, we might consider the following classes of models:

2.1 Deterministic vs. Stochastic

A stochastic model is one that uses *random variation.* On the other hand, in a deterministic model, there is no randomness. For example, a roll of the dice would use a stochastic model, while a model of how fast my cup of coffee cools down would not (therefore, my coffee cooling model would be deterministic- classically, the model would only involve the temperature of the coffee and the temperature of the environment). There may not be a clean division of categories here- for example, a model for a microphone may include deterministic portions (for the voice signal), and stochastic components (to model the electronic noise).

It is interesting to consider the following: Does a deterministic model necessarily produce results that are completely predictable through all time? Interestingly, the answer is: Maybe yes, Maybe no. Yes, in the theoretical sense- we might be able to show that there exists a single unique solution to our problem. No, in the practical sense that we might not actually be able to compute that solution. However, this does not mean that all is lost- we can get very good approximations over a finite time span (think of a weather model as an example). Of course, your deterministic system may be both completely predictable theoretically *and* practically.

Finally, think about the form of the final model when using a deterministic model versus a stochastic model. In the extreme cases, a deterministic model will be some set of functions and/or equations, while a stochastic model will try to describe the form of randomness that is observed, perhaps using the language of probabilities to describe the phenomenon.

2.2 Discrete vs. Continuous Time

In modeling an occurrence that depends on time, it might happen at discrete steps in time (like interest on my credit card), or in continuous time (like the temperature at my desk).

2.2.1 Modeling in Discrete Time

When modeling with difference equations, we are using two fundamental assumptions:

- Time is going by in discrete steps.
- The value of the process in the future is a function of a finite number of values from the past.

One way to realize this mathematically is the following general statement: Let a_n be a real number representing the state of the physical process at time unit n. Then

$$a_{n+1} = f(a_n, a_{n-1}, \ldots, a_{n-L})$$

Or, rather than modeling the states directly, we might model how the state *changes in time*:

$$a_{n+1} - a_n = f(a_{n-1}, \ldots, a_{n-L})$$

In either event, we will be left with determining the form for the function f and the length of the past, L.

We see these types of models in many places. In signals processing, models of this type are what make up the class of "filters". We see models of this type in population dynamics and statistics as well.

2.2.2 Modeling in Continuous Time

1. Modeling with Ordinary Differential Equations. In these models, we are assuming that time passes continually, and that the rate of change of the quantity of interest depends only on the quantity and current time. We capture these assumptions by the following general model, where $y(t)$ is the quantity of interest.

$$\frac{dy}{dt} = f(t, y)$$

Note that this says simply that the rate of change of the quantity y depends on the time t and the current value of y.

Let us consider an example we've seen in Calculus: Suppose that we assume that acceleration of a falling body is due only to the force of gravity (we'll measure it as feet/sec^2). Then we may write:

$$y'' = -16$$

We can solve this for $y(t)$ by antidifferentiation:

$$y' = -16t + C_1, \quad y(t) = -8t^2 + C_1 t + C_2$$

where C_1, C_2 are unknowns that are problem-specific.

To produce a more complex model, we might say that the rate of change depends not only on the quantity now, but also the value of the quantity in the past (for example, when regulating bodily functions the brain is reading values that are from the past). Such a model may take the following form, where $x(t)$ denotes the quantity of interest (such as the amount of oxygen in the blood):

$$\frac{dx}{dt} = f(x(t)) + g(x(t - \tau))$$

This is called a *delay differential equation*. One of the most famous of these models is the "Mackey-Glass" equation- You might look it up on the internet to see what the solution looks like!

2. Modeling with Partial Differential Equations. Sometimes, the quantity of interest may not be a function of time alone- perhaps it is a function of both time and position. In this case, the "ordinary" differential equation is replaced by a "partial" differential equation. For example, if u is a function of t (time) and x (position), we might write:

$$\frac{\partial u}{\partial t} = k \frac{\partial^2 u}{\partial x^2}$$

which might be interpreted to read: "The velocity of u at a particular time and position is proportional to its second spatial derivative.

If you're looking at this text at a more advanced level, you will learn more about modeling with ODEs and PDEs- for the beginning modeler, we'll wait on this.

2.3 Empirical vs. Analytical Modeling

"Empirical modeling" is modeling directly from data , rather than by some analytic process. In this case, our assumptions may take the form of a "model function" to which we will find unknown parameters. You've probably seen this before in articles where the researcher is fitting a line to data- in this example, we assume the model equation is given as $y = mx + b$, where m and b are the unknown parameters.

Consider, for example, the population of rabbits at time t.

- An Empirical Approach: Use the data directly to formulate model equations.
- An Analytical Approach: Start with some assumptions about the rabbit population, and build a difference or differential equation that captures those assumptions.

Note that with either approach, we still keep our rules of modeling in mind!

This text will first consider analytical models before going into some empirical modeling techniques. This is not because one is easier or harder than the other; empirical models are usually best expressed using a little linear algebra, which we will introduce as needed.

3 Finding an Answer

Once the general properties of your model have been set up, we will want to find answers to our questions. These might take the form of looking for a single analytic answer, optimization of a function, or performing a simulation.

3.1 An Analytic Answer

Our model may require us to solve one equation or a system of equations. We'll review the required topics from Calculus as we need them, but you might recall *Newton's Method*, which is a technique for solving $f(x) = 0$ for x:

1. Begin with a close estimate, x_0.
2. Iterate the following until you obtain the desired accuracy (or until the method fails):
$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

We'll practice this in the exercise section.

3.2 An Answer via Optimization

It may be required that to solve a model, we have to find the minimum or maximum of a function, and determine where the minimum or maximum occurs. To be specific about what we are asking, we will review some notation:

- To find the maximum value of a function, we'll write: $\max_x \ f(x)$

- To find *where* the maximum value of a function occurs, we'll write:

$$\arg\max_x \; f(x)$$

The "arg" stands for *argument*- The argument of a function is its input value.

- Similarly, the minimum and where the minimum occurs can be written (respectively) as:

$$\min_x f(x) \qquad \arg\min_x f(x)$$

Because optimization questions come up frequently in modeling, we will be considering these in some depth.

3.3 Simulations

Some models will only lead to answers by *computer simulation*. For example, predicting the weather is currently all done via computer simulations (do you recall your local weather person saying "The computer models tell us that this will occur"?). In order to perform these simulations and the other computations and graphs that are being considered, you will need to have access to some technology. A programmable calculator or a programming environment like *Matlab* will be a requirement- see your instructor for the specific technology you will use.

4 Exercises

1. Name three problems that might be modeled mathematically. Why do you think mathematics may provide a key to each solution? What is the added value in each case?

2. Consider the differential equation $\frac{dx}{dt} = x$. What is the solution to this equation? Translate this model into a difference equation. Compare the solutions and discuss.

3. Consider the *logistic equation* given by:

$$x_{n+1} = kx_n(1 - x_n)$$

   Compute the trajectory[2] of x and plot x_n versus n for the following conditions:

   (a) $x_0 = 0.6$, $k = 1.0$
   (b) $x_0 = 0.6$, $k = 3.0$
   (c) $x_0 = 0.6$, $k = 3.8$

[2]The trajectory (or orbit) is a listing of the values you get: $x_0, x_1, x_2, x_3, \ldots$.

Using the last conditions, change x_0 slightly to 0.60001, and plot the difference in the trajectory. What do you see over time?

The purpose of this exercise: Think about what we said about simple models producing complex behavior, and about the predictability of some solutions.

4. Recall that Newton's Method is used to solve $f(x) = 0$ for x. We gave the formula in the text, but here see if you can derive it using the following description:

   (a) Begin with an initial guess, x_0. Find the corresponding point, $(x_0, f(x_0))$ on the curve and draw a line from it to the x-axis.

   (b) *Exercise:* Find the $x-$intercept of this line algebraically. This will be x_1.

   Note that Newton's Method is itself a difference equation- that is, it can be written as:

$$x_{n+1} = g(x_n), \text{ with } g(x) = x - \frac{f(x)}{f'(x)}$$

   What would happen if I tried to use Newton's Method to solve the following for x: $x^2 + 1 = 0$. Try it and see! You might find it easiest to plot the trajectory of Newton's Method (x_n versus n), as we did in the logistic equation.

5. Consider the following numerical method for finding the minimum of a function:

   "At a point x, compute $f'(x)$. If $f'(x) > 0$, move x a slight distance backwards. If $f'(x) < 0$, move x a slight distance forwards. That is, create an orbit by moving in the opposite direction of the derivative:

$$x_{n+1} = x_n - hf'(x_n)$$

   where h is a small number."

   First, convince yourself that this is a reasonable thing to do by drawing a function and doing this graphically.

   Secondly, let's try this algorithm on a function and plot the trajectory, if

$$f(x) = x^4 - 2x^3 - x + 2, \quad x_0 = -0.5$$

   Try it for $h = 0.4, 0.3, 0.2, 0.1$. What do you see? Can you explain this?

6. In this exercise, we create a competition between three points in the plane, $(0, 0)$, $(1, 0)$ and $(0, 1)$. Each attracts a given point by first contracting it in the x and y directions, so that:

$$x_{n+1} = \frac{1}{2}x_n, \quad y_{n+1} = \frac{1}{2}y_n$$

but now choose one of the points at random. If point $(1, 0)$ is chosen, add $\frac{1}{2}$ to the x-coordinate. If point $(0, 1)$ is chosen, add $\frac{1}{2}$ to the y-coordinate. Program this model using a random initial point, and produce a plot of the orbit in the plane. Note that if $(0, 0)$ is chosen all the time, the orbit goes to that point- if $(1, 0)$ is chosen all the time, the orbit goes to that point- and the same for $(0, 1)$. Note that this produces our "competition".

Note: The purpose of this exercise is to get you to practice some basic programming and graphing- don't worry about the physical properties of the model!

7. (I) If you've had a course in ordinary differential equations, you're probably familiar with some of the standard techniques (like Runge-Kutta) for numerically computing a solution. You probably have not computed a solution for a delay differential equation- write about why it is more difficult to solve a differential equation with a time delay.