Introduction to Mathematical Modeling

Jonathan Goodman
Courant Institute of Mathematical Sciences, NYU

To the student

Mathematical modeling for us will mean using mathematical techniques to understand phenomena in the real world. To develop your modeling ability, I will present mathematical techniques and physical principles. This is material for you to learn. I will also focus on the more subtle art of making sensible physical and mathematical approximations. This is a skill to be practiced and nurtured. It requires intelligence, and a combination of skepticism and faith.

There are several reasons to build mathematical models. The most obvious is their predictive ability. We may want to know whether an newly designed airplane will fly before spending a billion dollars building a prototype. Equally important as motivation is human curiosity. Why does a vortex form when you drain a bathtub?[1] In both cases, the process starts with guesses at the important physical processes involved. It proceeds to write equations using the laws of physics. The last step is to figure what solutions of these equations look like. This may be done by finding a formula for the solution (rare), finding a good approximation, or by numerical computation or simulation.

To a large extent, modeling is the process of simplification and approximation. These go together, since the simpler model never tracks the more complicated one exactly. Finding the right level of complexity is an art form. To quote Albert Einstein: ”Everything should be a simple as possible, but no simpler.” It is common to make radical simplifications, particular when looking for a qualitative model. Among people who compute turbulent fluid flows, turbulence modeling is known as: ”replacing ignorance with fiction.”

An example of mathematical approximation

Throughout this class we will be ignoring “small” terms in equations as part of the model simplification process. I will start the class with an example of this, together with ways to assess the accuracy of the approximation and construct more accurate approximations to take into account the term we have dropped. The equation is

$$x + .1 \cdot x^2 = 2 \quad . \tag{1}$$

[1] There is a wonderful Simpsons episode that addresses this question.

The point is that because .1 is small, we may want to neglect it in first approximation. If we do this, we get

$$x \approx x_0 = 2 \ \ .$$

The first approximation is x_0, the second is x_1 and so on, like floors in a French building. In mathematics jargon x_0 is often called the "zeroth" approximation. To explore the accuracy of this approximation, we first reformulate (1) in a way that emphasizes (to math nurds) the importance of .1 being small:

$$x + \epsilon x^2 = 2 \qquad \text{with } \epsilon = .1. \tag{2}$$

More math jargon is the term "perturbation". We may regard the ϵx^2 term as a perturbation of the "unperturbed" equation $x = 2$. Then assessing the accuracy of the $x_0 = 2$ approximate solution is is the same as figuring out the effect of the perturbation.

Our first approach to this will be to use the approximation $x_0 = 2$ to estimate the size of the perturbation. After all, if $x \approx 2$ then $x^2 \approx 4$. With this, we get hopefully better approximation, x_1 by solving:

$$x_1 + \epsilon x_0^2 = 2 \ \ ,$$

which gives

$$x_1 = 2 - \epsilon x_0^2 = 2 - \epsilon \cdot 4 = 2 - .4 = 1.6 \ \ .$$

It is clear that we can continue this process. If x_1 is closer to x than x_0, then it will give a better estimate of the perturbation. With this, we could define a still better approximation, x_2, using x_1 to estimate the perturbation:

$$x_2 + \epsilon x_1^2 = 2 \ \ ,$$

so that

$$x_2 = 2 - .1 \cdot (1.6)^2 \approx 1.75 \ \ .$$

The actual "exact" value of x_2 is 1.744. I rounded the answer to $1.75 = 1\frac{3}{4}$ to indicate that I do not believe the last 4 is correct or even close. For example, I have no particular confidence that the exact answer, x, is less than 1.75. It is usual to report only those decimal digits you believe in. It is clear that you can continue this process of finding improved approximations. The first homework asks you to do so.

Review of Taylor series

Taylor series have many uses in pure and applied mathematics.[2] For us right now, they are a useful systematic way to construct mathematical approximations. The Taylor series[3] for a function $f(x)$ about a point, x_0, is

$$f(x) = f(x_0) + (x - x_0)\, f'(x_0) + (x - x_0)^2\, f''(x_0)/2 + \cdots + (x - x_0)^n\, f^{(n)}(x_0)/n! + \cdots \ \ .$$

[2]The technical journal published by the Courant Institute of Mathematical Sciences of NYU is called the *Communications of Pure and Applied Mathematics*.

[3]If you are rusty on Taylor series, I recommend the *Schaum's Outline of Calculus*. In general, I have found the *Schaum's Outline* series very useful for reviewing areas of mathematics.

Here, f' is the derivative of f, f'' is the second derivative, and $f^{(n)}$ is the n^{th} derivative. If $x - x_0$ is small, this gives a set of approximations of increasing accuracy:

$$\begin{aligned}
f_0(x) &= f(x_0) \\
f_1(x) &= f(x_0) + (x - x_0)\, f'(x_0) \\
f_2(x) &= f(x_0) + (x - x_0)\, f'(x_0) + (x - x_0)^2\, f''(x_0)/2 \\
& \text{ and so on.}
\end{aligned}$$

The first approximation just says that if x hasn't changed too much, maybe f hasn't changed much either. The f_1 approximation graphically represents the straight line tangent to the graph of $f(x)$ at the point x_0. It is easy to see in a graph that this is closer to the curved graph than the horizontal line approximation f_0. Often we call f_1 the "linear" approximation to $f(x)$ about x_0. However, there are pureists who prefer to call the function $f_1(x)$ *affine* because it is not linear in the sense of linear algebra. An affine function is linear in the linear algebra sense only of the graph passes through the origin. The f_2 approximation represents a parabola. If you draw carefully, you will see that the parabola is closer to the graph than the straight line corresponding to the linear (affine) approximation.

For example, if $f(x) = \sin(x)$ and $x_0 = \pi/3$ then

$$f(x_0) = \sin(x_0) = \sin(\pi/3) = \frac{\sqrt{3}}{2} = .8660 \ .$$

$$f'(x_0) = \cos(x_0) = \cos(\pi/3) = \frac{1}{2} = .5 \ .$$

$$f''(x_0) = -\sin(\pi/3) = -\frac{\sqrt{3}}{2} = -.8660 \ .$$

For $x = \pi/4$, $f(x) = \sin(x) = \sin(\pi/4) = 1/\sqrt{2} = .7071$, the Taylor series approximations are (with $\Delta x = x - x_0 = -\pi/12 = -.2618$)

$$\begin{aligned}
f_0 = .8660 & \qquad \text{error} = .8660 - .7071 = .1589. \\
f_1 = .8660 + \Delta x \cdot .5 = .7351 & \qquad \text{error} = .7351 - .7071 = .0280. \\
f_2 = .8660 + \Delta x \cdot .5 + \Delta x^2 \cdot (-.8660)/2 = .7054 & \qquad \text{error} = .7354 - .7071 = -.0017.
\end{aligned}$$

At least in this instance, the accuracy of the approximation improve as we take more terms.

The coefficient of $(x - x_0)^n$ is called the n^{th} Taylor series coefficient. Often it is possible to find the first few coefficients without having a formula for $f(x)$. This may allow us to approximate $f(x)$, at least for x values close enough to x_0. This is often possible when $f(x)$ is defined as the solution to an equation involving x in some way, as we shall see.

Back to the example

Let us see how these ideas work in the example of equation (2) above. The first thing we must do is switch all the letters. We want to find x for a given ϵ rather than f for a given x. Our function is $x(\epsilon)$ rather than $f(x)$. We will find the Taylor series coefficients for the expansion of $x(\epsilon)$ about $\epsilon = 0$. These will be called a_0, a_1, a_2, and so on. That is, we suppose that

$$x(\epsilon) = a_0 + \epsilon a_1 + \epsilon^2 a_2 + \cdots \quad .$$

The corresponding approximations are

$$x_0 = a_0 \ \ (= 2) \tag{3}$$
$$x_1 = a_0 + \epsilon a_1 \tag{4}$$
$$x_2 = a_0 + \epsilon a_1 + \epsilon^2 a_2 \tag{5}$$

and so on.

The coefficients a_0, a_1, $\cdots$, can be found by substitution of the approximations into the defining equation (2) and matching powers of ϵ one by one. For example, substituting (3) into (2) gives

$$a_0 + \epsilon a_0^2 = 2 \quad .$$

Since a_0 does not depend on ϵ, we cannot satisfy this equation exactly. Instead, we satisfy the part that does not depend on ϵ. This leads back to $a_0 = 2$.

The next coefficient can be found by substituting (4) into (2). This gives

$$a_0 + \epsilon a_1 + \epsilon(a_0^2 + 2\epsilon a_0 a_1 + \epsilon^2 a_1^2) = 2 \quad ,$$

or, after combining coefficients of like powers of ϵ,

$$a_0 + \epsilon(a_1 + a_0^2) + 2\epsilon^2 a_0 a_1 + \epsilon^3 a_1^2 = 2 \quad .$$

We choose a_0 and a_1 so that the lowest powers of ϵ are cancelled. In this case, those powers are $\epsilon^0 \equiv 1$ and $\epsilon^1 = \epsilon$. The ϵ^0 equation is formed by equating the coefficients of ϵ^2 on either side of the equation. The left is a_0 and the right side is 2. That gives

$$a_0 = 2 \quad .$$

The ϵ^1 equation is formed by equating coefficients of ϵ^1 on either side of the equation. The left side has $a_1 + a_0^2$ while the right side has 0 (the coefficient of ϵ in $2 = 2 + 0 \cdot \epsilon$ is 0). This gives

$$a_1 + a_0^2 = 0 \quad , \qquad \text{or} \qquad a_1 = -a_0^2 = -4 \; .$$

The final x_1 approximation, with $\epsilon = .1$ is

$$x \approx x_1 = a_0 + a_1 \cdot \epsilon = 2 + (-4) \cdot .1 = 1.6 \; .$$

This is the same as the x_1 we got in the earlier method.

The two methods give different x_2 approximations. In the present method, we have to compute, by squaring (5),

$$\begin{aligned} x_2^2 &= a_0^2 + 2\epsilon a_0 a_1 + \epsilon^2 a_1^2 + 2\epsilon^2 a_0 a_2 \\ & \quad 2\epsilon^3 a_1 a_2 + \epsilon^4 a_2^2 \ . \end{aligned}$$

We will soon examine how much of this laborious computation was actually necessary. For now, we simply substitute it into (2) and combine coefficients of like powers of ϵ:

$$\begin{aligned} a_0 &+ \epsilon(a_1 + a_0^2) + \epsilon^2(a_2 + 2a_0 a_1) \\ &+ \epsilon^3(a_1^2 + 2a_0 a_2) + \epsilon^4 2a_1 a_2 + \epsilon^5 a_2^2 = 2 \ . \end{aligned}$$

Now we have three unknown coefficients, a_0, a_1, and a_2, so we can match the first three powers of ϵ. This gives the a_0 and a_1 equations that we we got in constructing x_1. The ϵ^2 equation, which determines a_2, is

$$a_2 + 2a_0 a_1 = 0 \ , \quad \text{or} \quad a_2 = -2a_0 a_1 = (-2) \cdot 2 \cdot (-4) = 16 \ .$$

With this, the x_2 approximation is $x_2 = 2 - 4\epsilon + 16\epsilon^2$. Finally, with $\epsilon = .1$, we get

$$x \approx x_2 = 2 - 4 \cdot .1 + 16 \cdot .01 = 1.76 \ .$$