Fredy & Nadine Herrmann Institute of Earth Sciences

Mathematical Methods In Scientific Models

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Contents

List of Figures

Chapter 1

Small is NOT necessarily negligible

The standard practice in natural sciences to understand any physical, chemical or biological system is to somehow express it in the form of an equation. The equation to find the displacement s of a particle traveling along a straight line at a speed u and accelerating with time at a rate a is given by:

$$s = ut + \frac{1}{2}at^2 \tag{1.1}$$

where t is the time lapsed since the particle started moving. On the other hand, the decay of a radio active element like uranium can be quantified as:

$$N(t) = N_0 e^{-kt} \tag{1.2}$$

where N_0 is the initial number of atoms of uranium, k is the decay constant and $N(t)$ is the number of uranium atoms present after time t.

Such equations are a scientist's attempt to express any natural phenomena in terms of simple mathematical expressions often aimed at predicting the future state of any system. The general form of an equation is given by $f(x) = 0$. The left hand side (LHS) of the equation can consist of any number of terms. In context of determining the future state of a natural system, the terms on the LHS usually represent different mechanisms governing the system.

1.1 Finding approximate solutions to problems/equations that have no simple solutions

Ever so often, the scientific problems that we express as equations are not solvable. In that case one has to resort to some 'trickery' (a protocol) which makes the problem solvable. One such protocol which will be used extensively throughout this course can be summarised as follows:

1. Identify a (seemingly) small term in the problem/equation.
2. Solve the problem by setting the "small" term equal to 0.
3. Verify that the small term is indeed small by substituting the approximate solution we've found in the original problem and checking that the neglected term is indeed small.

The third step in the protocol ensures an apparent consistency. However, the reader should note that an apparently consistent solution may not be the real solution to the problem. We attempt to understand this protocol through a set of examples. We start the discussion by examining problems with known solutions in order to review the usefulness of the protocol.

1.1.1 Example 1: the protocol works!

Equations (1.3),(1.4) make up a set of linear algebraic equations with two unknowns. One learns to solve such equations in middle school but for the sake of illustrating our protocol we assume that we do not know how to solve this set of equations exactly.

$$x + 10y = 21 \tag{1.3}$$
$$5x + y = 7 \tag{1.4}$$

The first step of the protocol is to identify a small term, we assume that term x in (1.3) is small based on the values of the coefficients in this equation (1 compared to 10 and 21). As per the second item in our protocol, we set $x = 0$ in which case (1.3) simplifies to $10y \approx 21$ which yields the approximate solution $y = 2.1$. Substituting this value of y in (1.4) then yields the approximate value of $x = 0.98$. The third step is to check the apparent consistency of the solution. Substituting $x = 0.98$ and $y = 2.1$ on the LHS of (1.3) and (1.4) yields 21.98 and 7 respectively. Thus, we see that the condition of apparent consistency is also satisfied since the maximal relative error on the RHS is about 5% (i.e. 0.98/21).

If you solve this set of algebraic equations without following our protocol the exact solution is $x = 1$ and $y = 2$. In this particular case, our protocol has yielded approximate solutions that are close to the exact solutions 2.1 approximates 2 while 0.98 approximates 1 which falls within the anticipated 5% accuracy. However, this is not always the case as we'll see in the next example.

1.1.2 Example 2: the protocol does not work

Equations (1.5),(1.6) make up yet another set of linear equations with two variables.

$$0.01x + y = 0.1 \tag{1.5}$$
$$x + 101y = 11 \tag{1.6}$$

Following the protocol, as was done in the previous section, yields that the solution to the problem is $x = 0.9$ and $y = 0.1$. Despite satisfying the condition of apparent consistency, this approximate solution is very far away from the exact solution of $x = -90$ and $y = 1$. We now try to understand why does the protocol fail in this particular case. Set of equations (1.7), (1.8) is a generalization of the above set.

$$\epsilon x + y = 0.1 \tag{1.7}$$
$$x + 101y = 11 \tag{1.8}$$

Here ϵ is a real number. Solving (1.7) for x, yields $x = -\dfrac{0.9}{101\epsilon - 1}$. When $\epsilon \to 1/101$, the value of $x \to -\infty$. The coefficient in (1.5) is very close to 1/101 and that's why we get spurious solutions while employing the protocol.

1.1.3 Example 3: Wilkinson's polynomial

The Wilkinson's polynomial is a polynomial of degree 20, the roots of which are natural numbers $1, 2, 3, \ldots, 20$.

$$(x-1)(x-2)(x-3)\ldots(x-19)(x-20) = 0 \tag{1.9}$$

Let us add a tiny perturbation, $\epsilon \sim 10^{-10}$, to the Wilkinson's polynomial; the perturbed polynomial is given by:

$$(x-1)(x-2)(x-3)\ldots(x-19)(x-20) + \epsilon x^{19} = 0 \tag{1.10}$$

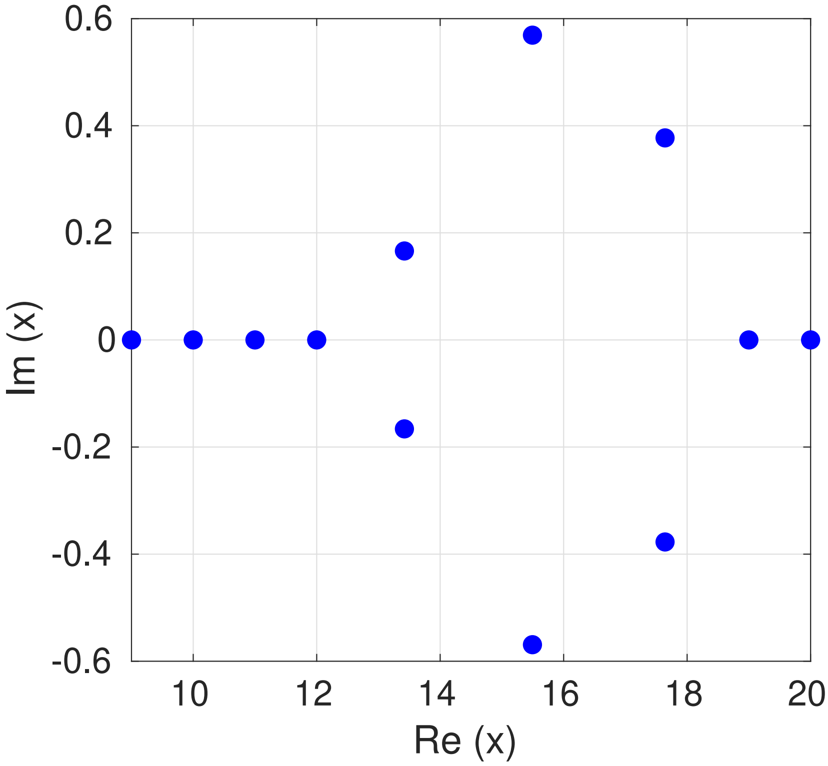

Figure 1.1: Roots of the perturbed Wilkinson polynomial on the complex plane for $\epsilon = 4\times 10^{-10}$. Roots smaller than 9 are not shown in the figure. [Adapted from Orszag and Bender (1978)]

As is illustrated in Figure 1.1, even such a 'small' perturbation ($\epsilon = 4 \times 10^{-10}$) renders a few roots of Wilkinson's polynomial (6 in this case), complex. Clearly, we need to develop a precise definition of what can be regarded as small.

1.2 Generalization: ill-posed equations/problems

In this section we develop a general framework to answer the question when a quantity appearing in a problem can be considered 'small'. To do the same, we assume that any problem we solve (differential equation, algebraic equation etc) is of the form $f(x) = 0$. The perturbed form of the same can be written as:

$$f[x(\epsilon), \epsilon] = 0. \tag{1.11}$$

We further assume

(a) for $\epsilon = 0$: $f[x(0), 0] = 0$

(b) for $0 < \epsilon \ll 1$: $f[x(0), \epsilon] - f[x(0), 0] \approx \epsilon \frac{\partial f}{\partial \epsilon}\Big|_{x(0)} := r$ is known (this is just the term added to the equation itself).

If ϵ is indeed small, we can approximate $f[x(\epsilon), \epsilon]$ as:

$$f[x(\epsilon), \epsilon] \approx f[x(0), 0] + \epsilon \frac{\partial f}{\partial x}\frac{\partial x}{\partial \epsilon}\Big|_{x(0)} + \epsilon \frac{\partial f}{\partial \epsilon}\Big|_{x(0)} \tag{1.12}$$

$$0 = 0 + \epsilon f_x . x_\epsilon + \epsilon f_\epsilon \tag{1.13}$$

$$\implies \epsilon x_\epsilon = -\frac{\epsilon f_\epsilon}{f_x} \tag{1.14}$$

Here $f_a \equiv \frac{\partial f}{\partial a}$. The quantity ϵx_ϵ is the measure of 'deviation' or change in the solution because of the perturbation and ϵf_ϵ is the measure of deviation in the equation itself. Since we know how much does the perturbation change the equation [through the condition of apparent consistency given by (b)] we can estimate the deviation in the solution as:

$$\frac{\epsilon x_\epsilon}{x} = -\frac{1}{f_x} \cdot \frac{r}{x} \tag{1.15}$$

The LHS is the relative error in the solution while the quantity $\frac{r}{x}$ on the RHS is the relative error in the equation caused by the addition of the ϵ term i.e. the perturbation term. For $f_x \ll 1$ the former (i.e. the error in the solution) is large even when $\frac{r}{x}$ (the error in the equation) is small. Thus, for the deviation or the error in the solution to be small for small ϵ, f_x has to be O(1).

1.3 Homework assignment 1

Water flowing from a small circular hole in a container has speed v which is approximately given by $v = 0.6\sqrt{2gh}$, where g is the gravitational acceleration and h is the height of the water above the hole. Let $A(h)$ be the area of the cross section at height h.

(a) Derive:

$$\frac{dh}{dt} = -0.6\frac{A(0)}{A(h)} \tag{1.16}$$

(b) Suppose that the actual shape of the container is approximated by $A(h) = h^c$, c is a constant. Solve the initial value problem. Discuss the apparent consistency of the approximation.

Bibliography

Orszag, S. and Bender, C. M. (1978), *Advanced mathematical methods for scientists and engineers*, McGraw-Hill New York, NY, USA.