Fredy & Nadine Herrmann Institute of Earth Sciences

Mathematical Methods In Scientific Models

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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:

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

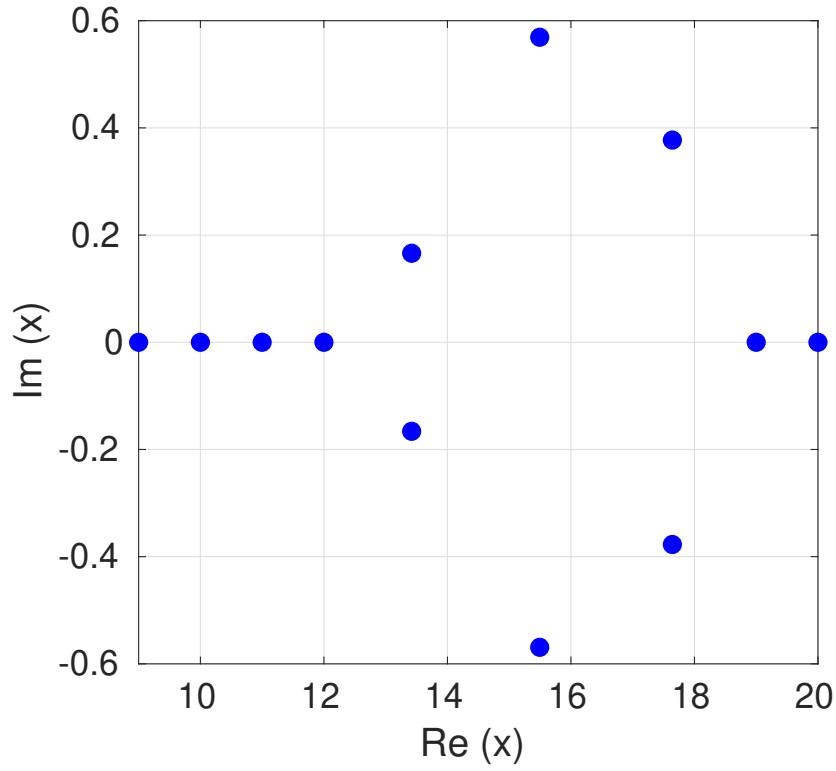

Figure 1.1: Roots of the perturbed Wilkinson's polynomial on the complex plane for $\epsilon = 4 \times 10^{-10}$. Roots smaller than 9 are not shown in the figure. [Adapted from Orszag and Bender (1978)]

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 $0 < \epsilon \ll 1$: $f[x(0), \epsilon] - f[x(0), 0] \approx \epsilon \dfrac{\partial f}{\partial \epsilon}\Big|_{x(0)} := r$ 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 $f_a \equiv \dfrac{\partial f}{\partial a}$. 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 $\dfrac{r}{x}$ 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 $\dfrac{r}{x}$ (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.

Chapter 2

Transformation to dimensionless variables

In the last chapter, we pointed out that natural scientists often cast the problems that they encounter into mathematical equations. However, more often than not, such equations (differential or algebraic) do not have an exact solutions and certain 'trickery' needs to be employed to obtain as reasonable a solution as possible. One such protocol we discussed is to assume that one (or more) of the terms in the equation is (are) preceded by a 'small' coefficient — ϵ, and solving the equation by setting $\epsilon = 0$. This protocol is neither unique nor perfect and we will continue to explore its different aspect throughout this course.

2.1 Tale of units

An equation usually comprises of a collection of variables upon which different operators e.g. addition, subtraction, differentiation act. For a natural scientists different operators need to conserve the 'units' in an equation. For instance,

$$\frac{du}{dt} - g + a = 0; \tag{2.1}$$

makes sense to a physicist only if u has the units of velocity and g and a have the units of acceleration. This way of thinking is quite convenient because by looking at the magnitude of different physical quantities, one can determine how much control does the quantity (and in turn the mechanism represented by that quantity) exercises on the system. However, our protocol relies on being able to identify small coefficients which may not be a trial task in a 'dimensional' equation for a variety of reasons, e.g. the coefficient itself may be composed of different physical quantities. To circumvent such issues, equations can be transformed from the dimensional framework to a non-dimensional one by scaling.

2.2 Scaling

To transform an equation from a dimensional framework to a non-dimensional one, we need to divide each of the variables (both dependent and independent) in the equation by a combination of parameters that has the same unit. Non-dimensionalizing equations not only makes it easier to compare different quantities in the equation but often also reduces the number of parameters in the problem.

2.2.1 Example 1: Friction-less motion of a fluid parcel

The equation of friction-less motion of a fluid parcel in 'natural coordinates' (Martin, 2013, refer to page 93-97) is given by:

$$\frac{v^2}{R} - fv = fv_g \tag{2.2}$$

where $v = |\vec{v}| > 0$ is the magnitude of velocity, f is the Coriolis frequency and v_g is the geostrophic velocity which satisfies the equation:

$$v_g = -\frac{1}{\rho f}\frac{\partial p}{\partial n}. \tag{2.3}$$

Here, p is the pressure and n is the perpendicular to the direction of motion. R is radius of curvature of parcel trajectory, $R > 0$ if $\hat{n}$ is directed toward the center of the curvature (counterclockwise flow) and $R < 0$ if $\hat{n}$ is directed away from the center (clockwise flow). Table 2.1 summarizes the dimensions of the variable v and the other parameters in equation (2.2).

Quantity	Dimensions
v	LT^{-1}
f	T^{-1}
v_g	LT^{-1}
R	L

Table 2.1: Dimensions of variables and parameters in (2.2)

Equations (2.2) can be scaled over either v_g or Rf since both have the dimensions of velocity. Let $\hat{v} = \dfrac{v}{Rf}$, therefore $v = \hat{v}Rf$. Substituting this in (2.2) yields:

$$\frac{\hat{v}^2(Rf)^2}{R} + f\hat{v}(Rf) = fv_g \tag{2.4}$$

$$\implies \underbrace{\hat{v}^2}_{\text{dimensionless}} + \underbrace{\hat{v}}_{\text{dimensionless}} = \underbrace{\frac{v_g}{Rf}}_{\text{dimensionless}} \tag{2.5}$$

Substituting $\hat{v} = R_0$ and $\dfrac{v_g}{Rf} = R_{0g}$ in (2.5) yields:

$$R_0^2 + R_0 = R_{0g} \tag{2.6}$$

which is an equation with only one non-dimensional parameter. Figure 2.1 illustrates the solutions of (2.6) for different values of R_{0g}. As an exercise the reader should try and interpreting what these different R_{0g} regimes represent in the context of dynamic meteorology.

Equation (2.2) can be scaled over v_g instead of Rf to yield:

$$\frac{\hat{v}^2(v_g)^2}{R} + f\hat{v}(v_g) = fv_g \tag{2.7}$$

$$\implies \frac{v_g}{fR}\hat{v}^2 + \hat{v} = 1 \tag{2.8}$$

Substituting $\frac{v_g}{fR} = R_{0g}$ yields:

$$R_{og}\hat{v}^2 + \hat{v} = 1 \tag{2.9}$$

For $R_{0g} \ll 1$ i.e. for $R \gg \dfrac{v_g}{f}$, (2.9) yields the geostrophic solution. It is rather non-trivial to obtain this solution from (2.6) because the parameter R is used in the scaling itself. **It is advised not to use the parameter which needs to be varied as a scale**.

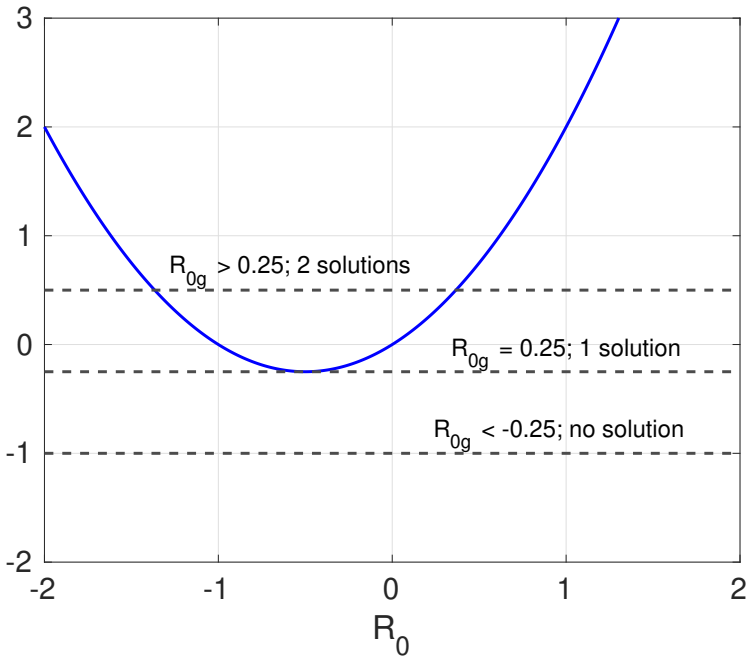

Figure 2.1: Solutions of (2.6) for different R_{0g} regimes.

As is evident from (2.5) and (2.8), there are two scales for v. Likewise, in any problem there are multiple combination of parameters over which the dimensional variables can be scaled, however, not every scaling yields solvable non-dimensional equations. We explore this in our next example.

2.2.2 Example 2: Problem of a projectile

We explore the dynamics of a small projectile launched upwards from ground with a vertical velocity of v. The equation of motion for that projectile is given by:

$$\frac{d^2z}{dt^2} = -g\frac{a^2}{(a+z)^2} \tag{2.10}$$

where z is the displacement of the projectile from the surface ($z = 0$) and g is the gravitational acceleration at the surface and a is the radius of Earth. The initial conditions associated with (2.10) are:

$$z(0) = 0 \quad \text{and} \quad \frac{dz}{dt}\Big|_{z=0} = 0. \tag{2.11}$$

There are two variables z (dependent) and t (independent) and three parameters a, g and v in (2.10). The dimensions of z, t, a, g and v are L, T, L, LT^{-2} and LT^{-1} respectively.

The classical approach to solve this problem is to assume that $z \ll a$ i.e. the gravitational acceleration does not vary much with the height of the projectile from the surface and solve for z as a function of t which yields:

$$z = vt - \frac{1}{2}gt^2 \tag{2.12}$$

The maximum height for the projectile is $z_{max} = \dfrac{v^2}{2g}$. For $z \ll a$ to be a valid assumption, $z_{max} \ll a \implies v \ll \sqrt{2ag}$. We now try to reach this conclusion in the non-dimensional framework.

Substituting $\hat{z} = \dfrac{z}{a}$ and $\hat{t} = \dfrac{t}{a/v}$ in (2.10) yields:

$$\begin{aligned}
\frac{1}{(a/v)^2}\frac{d^2}{d\hat{t}^2}(a\hat{z}) &= -g\frac{a}{(a+a\hat{z})^2} \\
\frac{v^2}{a}\frac{d^2\hat{z}}{d\hat{t}^2} &= -\frac{g}{(1+\hat{z})^2} \\
\frac{d^2\hat{z}}{d\hat{t}^2} &= -\frac{ag}{v^2}\frac{1}{(1+\hat{z})^2}
\end{aligned}$$

Substituting $\dfrac{v^2}{ag} = \epsilon$ yields:

$$\epsilon\frac{d^2\hat{z}}{d\hat{t}^2} = -\frac{1}{(1+\hat{z})^2} \tag{2.13}$$

The initial conditions can be rewritten as $\hat{z}(0) = 0$ and $\left.\dfrac{d\hat{z}}{d\hat{t}}\right|_{\hat{z}=0} = 1$. Clearly, for $\epsilon = 0$, the equation is not solvable. We need to find the appropriate scaling which yields a solvable equation. Table 2.2 provides a summary of all the non-dimensionalized versions of (2.10). Clearly, the non-dimensional equation is solvable only when time is scaled over v/g and length is scaled over v^2/g.

Time scale Length scale	a/v a	$\sqrt{a/g}$ a	v/g a
ODE	$\epsilon\dfrac{d^2\hat{z}}{d\hat{t}^2} = -\dfrac{1}{(1+\hat{z})^2}$	$\dfrac{d^2\hat{z}}{d\hat{t}^2} = -\dfrac{1}{(1+\hat{z})^2}$	$\dfrac{d^2\hat{z}}{d\hat{t}^2} = -\dfrac{\epsilon}{(1+\hat{z})^2}$
ICs	$\hat{z}(0) = 0$ & $\left.\dfrac{d\hat{z}}{d\hat{t}}\right\|_{\hat{z}=0} = 1$	$\hat{z}(0) = 0$ & $\left.\dfrac{d\hat{z}}{d\hat{t}}\right\|_{\hat{z}=0} = \epsilon^{1/2}$	$\hat{z}(0) = 0$ & $\left.\dfrac{d\hat{z}}{d\hat{t}}\right\|_{\hat{z}=0} = \epsilon$
Time scale Length scale	a/v v^2/g	$\sqrt{a/g}$ v^2/g	v/g v^2/g
ODE	$\epsilon^2\dfrac{d^2\hat{z}}{d\hat{t}^2} = -\dfrac{1}{(1+\epsilon\hat{z})^2}$	$\epsilon\dfrac{d^2\hat{z}}{d\hat{t}^2} = -\dfrac{1}{(1+\epsilon\hat{z})^2}$	$\dfrac{d^2\hat{z}}{d\hat{t}^2} = -\dfrac{1}{(1+\epsilon\hat{z})^2}$
ICs	$\hat{z}(0) = 0$ & $\left.\dfrac{d\hat{z}}{d\hat{t}}\right\|_{\hat{z}=0} = \dfrac{1}{\epsilon}$	$\hat{z}(0) = 0$ & $\left.\dfrac{d\hat{z}}{d\hat{t}}\right\|_{\hat{z}=0} = \dfrac{1}{\epsilon^{1/2}}$	$\hat{z}(0) = 0$ & $\left.\dfrac{d\hat{z}}{d\hat{t}}\right\|_{\hat{z}=0} = 1$

Table 2.2: Summary of all non-dimensionalized versions of (2.10); $\epsilon = v^2/ag$.

2.3 Conclusion: Why do we scale?

1. Scaling the dimensional equation(s) often reduces the number of parameters in the problem. We note that it is not necessary that the parameters only appear in the equations. They can appear in the initial/boundary condition(s) as well.

2. Scaling ensures that the size of the term in the problem (i.e. the controlling mechanism of a system) is accurately estimated by its coefficient.

3. Scaling yields an acceptable known solution to the problem when one of the non-dimensional parameters is set equal to 0. This usually represents one of the asymptotic limits associated with the problem at hand.

2.4 Homework assignment 2

Verify that all the ODEs listed in Table 2.2 are correct, by non-dimensionalizing (2.10) using the different scales given in the table.

Chapter 3

Regular perturbation methods

Natural scientists often express problems in dynamics (particle motion, flow of geophysical fluids, chemical kinetics) as differential equations. However, only a handful of these equations can be solved (integrated) to obtain exact analytical solutions. To be precise the number of solvable equations can be classified into two categories:

a) linear[1], ordinary differential equations (ODEs) with constant coefficient with simple initial/boundary conditions and

b) homogeneous partial differential equations (some extension to in-homogeneous equations also exist).

Over time, mathematicians have developed several methods which can be employed to obtain solutions to these 'unsolvable' differential equations. One category of such methods are the perturbation methods which will be discussed at length through this course. At its crux, any perturbation method/technique involves three steps, i) finding the exact solution to a simpler version of the problem, ii) assuming that the solution to the original problem is a small 'perturbation' added to the simple solution and iii) estimating the perturbation terms.

3.1 Regular perturbation

We illustrate the applicability of perturbation methods by solving the following algebraic equation using the regular perturbation method:

$$x^3 - (4+\epsilon)x + 2\epsilon = 0 \tag{3.1}$$

where $\epsilon = 0.001$. For $\epsilon = 0$, the solutions to (3.1) are $x = \{-2, 0, 2\}$. We assume that for $\epsilon \neq 0$, the solution to (3.1) is of the form $x = x_i + \delta$ where x_i is the solution to the simpler equation i.e. the equation with $\epsilon = 0$. Since $x_i + \delta$ is a solution to (3.1):

$$\begin{aligned} (x_i+\delta)^3 - (4+\epsilon)(x_i+\delta) + 2\epsilon &= 0 \\ x_i^3 + 3x_i^2\delta + 3x_i\delta^2 + \delta^3 - (4x_i + \epsilon x_i + 4\delta + \epsilon\delta) + 2\epsilon &= 0 \end{aligned} \tag{3.2}$$

As per our assumptions, $\delta \sim \epsilon \ll 1$ and hence the higher order terms in (3.2) can be safely neglected to yield:

$$x_i^3 + 3x_i^2\delta - 4x_i - \epsilon x_i - 4\delta + 2\epsilon = 0. \tag{3.3}$$

Substituting $x_i = -2$ in (3.3) yields $\delta = -\dfrac{\epsilon}{2}$, thus one of the (approximated) roots to (3.1) is $x = -2 + \dfrac{0.001}{2} = 1.9995$. The other roots can be calculated similarly.

[1] A differential equation is linear if the all the derivatives appearing in the equation have power one.

3.2 Homework assignment 3

Calculate the root by neglecting $O(3)$ or higher terms in (3.2). How many values of δ do you obtain? Are all the values acceptable perturbations to the simple solution?

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