1.1 Differential Equations

Differential equations are often used to describe natural processes. Consider the elementary problem of finding the temperature in a bar where one end, at $r = r_A$, is held at constant temperature T_A, and at the other end, $r = r_B$, it is held at temperature T_B. The only mechanism for heat transfer within the bar is by molecular diffusion, so that the governing equation is,

{temper1}
$$\kappa \frac{d^2T}{dr^2} = 0 \tag{1.1}$$

subject to the boundary conditions,

{temper2}
$$T(r_A) = T_A,\ T(r_B) = T_B. \tag{1.2}$$

Eq. (1.1) is so simple we can write its solution in a number of different ways. One form is,

$$T(r) = a + br, \tag{1.3}$$

where a, b unknown parameters, until some additional information is provided. Here the additional information is contained in the boundary conditions (1.2), and with two parameters to be found, there is just sufficient information, and

$$T(r) = \frac{r_B T_A + r_A T_B}{r_B - r_A} + \left(\frac{T_B - T_A}{r_B - r_A}\right) r, \tag{1.4}$$

a straight line. Such problems, or analogues for much more complicated systems, are sometimes called "forward" or "direct" and they are "well-posed": exactly enough information is available to produce a unique solution (easily proved here, not so easily in other cases). If there are small perturbations in T_i, or r_i, then the solution changes only slightly—it is also stable and differentiable. This sort of problem and its solution is what is generally taught starting in elementary science courses.

On the other hand, the problems one encounters in actually doing science differ significantly—both in the questions being asked, and in the information available. A very large number of possibilities presents itself:

1. One or both of the boundary values T_A, T_B is known from measurements; they are thus given as $T_A = T_A^{(c)} \pm \Delta T_A$, $T_B = T_B^{(c)} \pm \Delta T_B$, where the $\Delta T_{A,B}$ are an estimate of the possible inaccuracies in the theoretical values $T_i^{(c)}$. (Exactly what that might mean is taken up later.)

2. One or both of the positions, $r_{A,B}$ is also the result of measurement and are of the form $r_{A,B}^{(c)} \pm \Delta r_{A,B}$.

3. T_B is missing altogether, but is known to be positive, $T_B > 0$.

4. One of the boundary values e.g., T_B, is unknown, but an interior value $T_{int} = T_{int}^{(c)} \pm \Delta T_{int}$ is provided instead. Perhaps many interior values are known, but none of them perfectly.

Other possibilities exist. But even this short list raises a number of interesting, practical problems. One of the themes of this book is that almost nothing in reality is known perfectly. It is possible that $\Delta T_A, \Delta T_B$ are very small; but as long as thye are not actually zero, there is no longer any possibility of finding a single unique solution.

Many variations on this model and theme arise in practice. Suppose the problem is made slightly more interesting by introducing a "source" $S_T(r)$, so that the temperature field is thought to satisfy the equation,

$$\frac{d^2T(r)}{dr^2} = S_T(r), \tag{1.5}$$ {temper3}

along with its boundary conditions, producing another conventional forward problem. One can convert (1.5) into a different problem by supposing that one knows $T(r)$, and seeks $S_T(r)$. Such a problem is even easier to solve than the conventional one: differentiate T twice. Because convention dictates that the "forward problem" involves the determination of $T(r)$ from a known $S_T(r)$ and boundary data, this latter problem might be labelled as an "inverse" one—simply because it contrasts with the conventional formulation.

In practice, a whole series of new problems can be raised: suppose $S_T(r)$ is imperfectly known. How should one proceed? If one knows $S_T(r)$ and $T(r)$ at a series of positions $r_i \neq r_A, r_B$, could one nonetheless deduce the boundary conditions? Could one deduce $S_T(r)$ if it were not known at these interior values?

$T(r)$ has been supposed to satisfy the differential equation (1.1). For many purposes, it is helpful to reduce the problem to one that is intrinsically discrete. One way to do this would be to expand the solution in a system of polynomials,

$$T(r) = \alpha_0 r^0 + \alpha_1 r^1 + ... + \alpha_n r^n, \tag{1.6}$$

and

$$S_T(r) = \beta_0 r^0 + \beta_1 r^1 + ... + \beta_n r^n \tag{1.7}$$

where the β_i would conventionally be known, and the problem has been reduced from the need to find a function $T(r)$ defined for all values of r, to one in which only the finite number of parameters $\alpha_i,\ 0 \leq i \leq n$ must be found.

An alternative discretization is obtained by using the coordinate r. Divide the interval $r_A = 0 \leq r \leq r_B$ into $N-1$ intervals of length Δr, so that $r_B = (N-1)\,\Delta r$. Then, taking a simple two-sided difference:

$$\begin{aligned} T(2\Delta r) - 2T(\Delta r) + T(0) &= (\Delta r)^2 S_T(0) \\ T(3\Delta r) - 2T(2\Delta r) + T(1\Delta r) &= (\Delta r)^2 S_T(1\Delta r) \\ &\cdot \\ &\cdot \\ T((N-1)\Delta r) - 2T((N-2)\Delta r) + T((N-3)\Delta r) &= (\Delta r)^2 S_T((N-2)\Delta r) \end{aligned} \tag{1.8}$$

If one counts the number of equations in (1.8) it is readily found that there are $N-2$ of them, but with a total of N unknown $T(p\Delta r)$. The two missing pieces of information are provided by the two boundary conditions $T(0\Delta r) = T_0,\ T((N-1)\Delta r) = T_{N-1}$. Thus the problem of solving the differential equation has been reduced to finding the solution of a set of ordinary linear simultaneous algebraic equations, which we will write, in the notation of Chapter 2 as,

{equal1}
$$\mathbf{A}\mathbf{x} = \mathbf{b}, \tag{1.9}$$

where $\mathbf{A}$ is a square matrix, $\mathbf{x}$ is the vector of unknowns $T(p\Delta t)$, and $\mathbf{b}$ is the vector of values $\mathbf{q}(p\Delta t)$, and of boundary values. The list above, of variations, e.g., where a boundary condition is missing, or where interior values are provided instead of boundary conditions, become statements then about having too few, or possibly too many, equations for the number of unknowns. Uncertainties in the T_i or in the $q(p\Delta r)$ become statements about having to solve simultaneous equations with uncertainties in some elements. That models, even nonlinear ones, can be reduced to sets of simultaneous equations is the unifying theme of this book. One might need truly vast numbers of grid points, $p\Delta r$, or polynomial terms, and ingenuity in the formulation to obtain adequate accuracy, but as long as the number of parameters, $N < \infty$, one has achieved a great, unifying simplification.

Consider a bit more interesting ordinary differential equation, that for the simple mass-spring oscillator,

{ms1}
$$m\frac{d^2\xi(t)}{dt^2} + \varepsilon\frac{d\xi(t)}{dt} + k_0\xi(t) = S_\xi(t), \tag{1.10}$$

where m is mass, k_0 is a spring constant, and ε is a dissipation parameter. Although the equation is slightly more complicated than is (1.5), and we have relabelled the independent variable as t (to suggest time), rather than as r, there really is no fundamental difference. This differential equation can also be solved in any number of ways. As a second order equation, it is well-known that one must provide two extra conditions to have enough information to have a unique

solution. Typically, there are *initial* conditions, $\xi(0), d\xi(0)/dt$—a position and velocity, but there is nothing to prevent us from assigning two end conditions, $\xi(0), \xi(t = t_f)$, or even two velocity conditions $d\xi(0)/dt, d\xi(t_f)/dt$, etc.

If we naively discretize (1.10) as we did the straight-line equation, we have,

$$\xi(p\Delta t + \Delta t) - \left(2 - \frac{\varepsilon \Delta t}{m} - \frac{k(\Delta t)^2}{m}\right) \xi(p\Delta t) - \left(\frac{\varepsilon \Delta t}{m} - 1\right) \xi(p\Delta t - \Delta t) \qquad (1.11)$$
$$= (\Delta t)^2 \frac{S_\xi(p\Delta t)}{m}, \quad 2 \leq p \leq N-1$$

which is another set of simultaneous equations as in (1.9) in the unknown $\xi(p\Delta t)$; an equation count again would show that there are two fewer equations than unknowns—corresponding to the two boundary or two initial conditions. In Chapter 2, several methods will be developed for solving sets of simultaneous linear equations, even when there are apparently too few or too many of them. In the present case, if one were given $\xi(0), \xi(1\Delta t)$, Eq. (1.11) could be stepped forward in time, generating $\xi(3\Delta t), \xi(4\Delta t)$, ...,$\xi((N-1)\Delta t)$. The result would be identical to the solution of the simultaneous equations—but with far less computation.

But if one were given $\xi((N-1)\Delta t)$ instead of $\xi(1\Delta t)$, such a simple time-stepping rule could no longer be used. One would have a similar difficulty if $q(j\Delta t)$ were missing for some j, but instead one had knowledge of $\xi(p\Delta t)$, for some p. Looked at as a set of simultaneous equations, there is no conceptual problem: one simply solves it, all at once, by Gaussian elimination or equivalent. There *is* a problem only if one sought to time-step the equation forward, but without the required second condition at the starting point—there would be inadequate information to go forward in time. Many of the methods explored in this book are ways to solve simultaneous equations while avoiding the need for all-at-once brute force solution. Nonetheless, one is urged to always recall that most of the interesting algorithms are just clever ways of solving large sets of such equations.