Chapter 1

Introduction

The most powerful insights into the behavior of the physical world are obtained when direct observations are well described by a theoretical framework that is then available for predicting new phenomena or new observations. An example is the observed behavior of radio signals and their extremely accurate description by the Maxwell equations of electromagnetic radiation. Other such examples include planetary motions as described by Newtonian mechanics, or the movement of the atmosphere and ocean as described by the equations of fluid mechanics, or the propagation of seismic waves in the earth as described by the elastic wave equations. To the degree that the theoretical framework supports, and is supported by, the observations one develops sufficient confidence to calculate similar phenomena in previously unexplored domains or to make predictions of future behavior (the position of the moon 1000 years, or the climate state of the earth 100 years, in the future).

Developing a coherent view of the physical world requires some mastery, therefore, of both a framework, and of the meaning and interpretation of real data. Conventional scientific education, at least in the physical sciences, puts a heavy emphasis on learning how to solve appropriate differential and partial differential equations (Maxwell, Schrodinger, Navier-Stokes, etc.). One learns which problems are "well-posed", how to construct solutions either exactly or approximately, and how to interpret the results. Much less emphasis is placed on the problems of understanding the implications of data, which are inevitably imperfect—containing noise of various types, are often incomplete, and possibly inconsistent.

Many interesting problems arise in using observations in conjunction with theory. In particular, one is driven to conclude that there are no well-posed problems outside of textbooks, that stochastic elements are inevitably present and must be confronted, and that more generally, one must make inferences about the world from data that are necessarily always incomplete. The main purpose of this introductory chapter is to provide some comparatively simple ex-

amples of the type of problems one confronts in practice, and for which many interesting and useful tools exist for their solution. In an older context, this subject was called the "calculus of observations."[2]

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,

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

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.

1.2 Partial Differential Equations

Finding the solutions of linear differential equations is equivalent, when discretized, to solving sets of simultaneous linear algebraic equations. Unsurprisingly, the same is true of partial differential equations. As an example, consider a very familiar problem:

Solve

$$\nabla^2 \phi = \rho, \tag{1.12}$$ {eq:13001}

for ϕ, given ρ, in the domain $\mathbf{r} \in D$, subject to the boundary conditions $\phi = \phi_0$ on the boundary ∂D, where $\mathbf{r}$ is a spatial coordinate of dimension greater than 1.

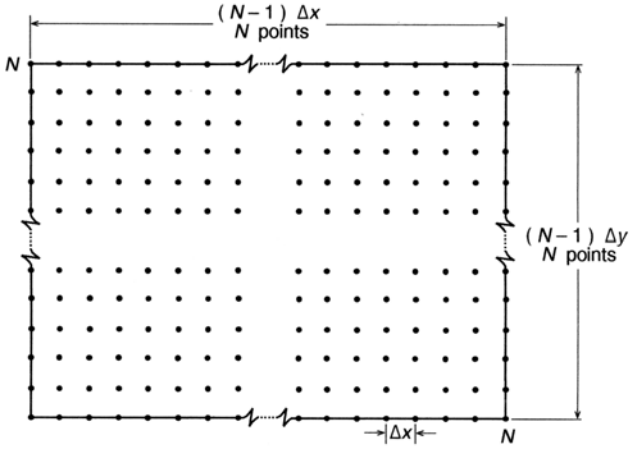

Figure 1.1: Square, homogeneous grid used for discretizing the Laplacian, thus reducing the partial differential equation to a set of linear simultaneous equations.

{grid1.tif}

This statement is the Dirichlet problem for the Laplace-Poisson equation, whose solution is well-behaved, unique, and stable to perturbations in the boundary data, ϕ_0, and the source or forcing, ρ. Because it is the familiar boundary value problem, it is by convention again labeled a forward or direct problem. Now consider a different version of the above:

Solve (1.12) for ρ given ϕ in the domain D.

This latter problem is even easier to solve than the forward problem: merely differentiate ϕ twice to obtain the Laplacian, and ρ is obtained directly from (1.12). Because the problem as stated is inverse to the conventional forward one, it is labeled, as with the ordinary differential equation, an *inverse problem*. It is inverse to a more familiar boundary value problem in the sense that the usual unknowns ϕ have been inverted or interchanged with (some of) the usual knowns ρ. Notice that both forward and inverse problems, as posed, are well-behaved and produce uniquely determined answers (ruling out mathematical pathologies in any of ρ, ϕ_0, ∂D, or ϕ). Again, there are many variations possible: one could, for example, demand computation of the boundary conditions, ϕ_0, from given information about some or all of ϕ, ρ.

Write the Laplace-Poisson equation in finite difference form for two Cartesian dimensions:

{eq:13002}

$$\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j} + \phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1} = (\Delta x)^2 \rho_{ij}, \quad i, j \in D, \tag{1.13}$$

with square grid elements of dimension Δx. To make the bookkeeping as simple as possible, suppose the domain D is the square $N \times N$ grid displayed in Figure 1.1, so that ∂D is the four

line segments shown. There are $(N-2)\times(N-2)$ interior grid points, and Equations (1.13) are then $(N-2)\times(N-2)$ equations in N^2 of the ϕ_{ij}. If this is the forward problem with ρ_{ij} specified, there are fewer equations than unknowns. But if we append to (1.13) the set of boundary conditions:

$$\phi_{ij} = \phi^0_{ij}\,, \quad i,\, j \in \partial D\,, \tag{1.14}$$ {eq:13003}

there are precisely $4N-4$ of these conditions, and thus the combined set (1.13) plus (1.14), which we write again as (1.9) with,

$$\mathbf{x} = \mathrm{vec}\{\phi_{ij}\} = \begin{bmatrix} \phi_{11} \\ \phi_{12} \\ . \\ . \\ \phi_{NN} \end{bmatrix}, \qquad \mathbf{b} = \mathrm{vec}\left\{\rho_{ij}, \phi^0_{ij}\right\} = \begin{bmatrix} \rho_{2,N+1} \\ \rho_{2,N+2} \\ . \\ . \\ \rho_{N-2,N-2} \\ \phi^0_{11} \\ . \\ \phi^0_{N,N} \end{bmatrix},$$

a set of $M = N^2$ equations in $M = N^2$ unknowns. (The operator, vec, forms a column vector out of the two-dimensional array ϕ_{ij}.) The nice properties of the Dirichlet problem can be deduced from the well-behaved character of the matrix $\mathbf{A}$. Thus the forward problem corresponds directly with the solution of an ordinary set of simultaneous algebraic equations.[3] One complementary inverse problem says: "Using (1.9) compute ρ_{ij} and the boundary conditions, given ϕ_{ij}," an even simpler computation—it involves just multiplying the known $\mathbf{x}$ by the known matrix $\mathbf{A}$.

But now let us make one small change in the forward problem, changing it to the Neumann one:

Solve,

$$\nabla^2\phi = \rho, \tag{1.15}$$ {eq:13005}

for ϕ, given ρ, in the domain $\mathbf{r} \in D$ subject to the boundary conditions $\partial\phi/\partial\hat{\mathbf{m}} = \phi'_0$ on the boundary ∂D, where $\mathbf{r}$ is again the spatial coordinate and $\hat{\mathbf{m}}$ is the unit normal to the boundary.

This new problem is another classical, much analyzed forward problem. It is, however, well-known that the solution is indeterminate up to an additive constant. This indeterminacy is clear

in the discrete form: Equations (1.14) are now replaced by

$$\phi_{i+1,j} - \phi_{i,j} = \phi'^{0}_{ij}, \qquad i,\, j \in \partial D' \tag{1.16}$$ {eq:13006}

etc., where $\partial D'$ represents the set of boundary indices necessary to compute the local normal derivative. There is a new combined set:

$$\mathbf{A}\mathbf{x} = \mathbf{b}_1,\ \mathbf{x} = \mathrm{vec}\left\{\phi_{ij}\right\},\ \mathbf{b}_1 = \mathrm{vec}\left\{\rho_{ij}, \phi'^{0}_{ij}\right\} \tag{1.17}$$ {eq:13007}

Because only *differences* of the ϕ_{ij} are specified, there is no information concerning the absolute value of $\mathbf{x}$. When we obtain some machinery in Chapter 2, we will be able to demonstrate automatically that even though (1.17) appears to be M equations in M unknowns, in fact only $M-1$ of the equations are independent, and thus the Neumann problem is an underdetermined one. This property of the Neumann problem is well-known, and there are many ways of handling it, either in the continuous or discrete forms. In the discrete form, a simple way is to add one equation setting the value at any point to zero (or anything else). Notice, however, that in all cases, the inverse problem of determining $\mathbf{b}_1$ from $\mathbf{x}$ remains simple and well-posed.

1.3 More Examples

e:boxmodel1} *A Tracer Box Model*

In scientific practice, one often has observations of elements of the solution of the differential system or other model. Such situations vary enormously in the complexity and sophistication of both the data and the model. A useful and interesting example of a simple system, with applications in many fields, is one in which there is a large reservoir (Figure 1.2) connected to a number of source regions which provide fluid to the reservoir. One would like to determine the
getracerfig} rate of mass transfer from each source region to the reservoir.

We suppose that some chemical tracer or dye, C_0 is measured in the reservoir, and that the concentrations of the dye, C_i, in each source region are known. Let the unknown transfer rates be J_{i0} (transfer from source i to reservoir 0). Then we must have,

$$C_1 J_{10} + C_2 J_{20} + ... + C_N J_{N0} = C_0 J_{0\infty}, \tag{1.18}$$ {tracer1}

which says that for a steady-state, the rate of transfer in, must equal the rate of transfer out (written $J_{0\infty}$). To conserve mass,

$$J_{10} + J_{20} + ... + J_{N0} = J_{0\infty}. \tag{1.19}$$ {tracer2}

This model has produced for us two equations in $N+1$ unknowns, $[J_{10}, J_{20}, ...J_{N0}, J_{0\infty}]$ which evidently is insufficient information if $N > 1$. The equations have also been written as though

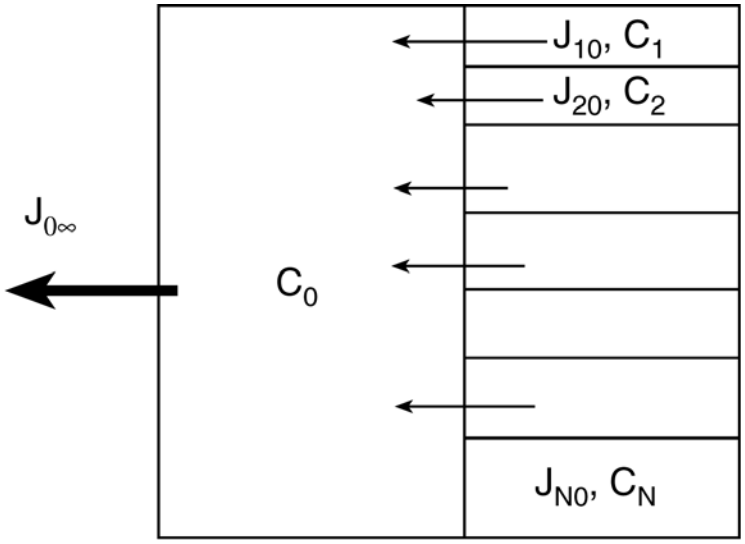

Figure 1.2: A simple reservoir problem in which there are multiple sources of flow, at rates J_{i0}, each carrying an identifiable property C_i, perhaps a chemical concentration. In the forward problem, given J_{i0}, C_i one could calculate C_0. One form of inverse problem provides C_0 and the C_i and seeks the values of J_{i0}.

{reserv1.tif}

everything were perfect. If, for example, the tracer concentrations C_i were measured with finite precision and accuracy (they always are), one might try to accommodate the resulting inaccuracy as,

$$C_1 J_{10} + C_2 J_{20} + ... + C_N J_{N0} + n = C_0 J_{0\infty} \tag{1.20}$$

{tracer3}

where n represents the resulting error in the equation. Its introduction, of course, produces another unknown. If the reservoir were capable of some degree of storage or fluctuation in level, one might want to introduce an error term into (1.19) as well. One should also notice, that as formulated, one of the apparently infinite number of solutions to Eqs. (6.1, 1.19) includes $J_{i0} = J_{0\infty} = 0$—no flow at all. More information is required if this null solution is to be excluded.

To make the problem slightly more interesting, suppose that the tracer C is radioactive, and decays with a decay constant λ. Eq. (6.1) becomes

$$C_1 J_{10} + C_2 J_{20} + ... + C_N J_{N0} - C_0 J_{0\infty} = -\lambda C_0 \tag{1.21}$$

Now if $C_0 > 0$, the zero solution for J_{ij} is no longer possible, but we still have many more unknowns than equations. These equations are once again in the canonical linear form $\mathbf{Ax} = \mathbf{b}$.

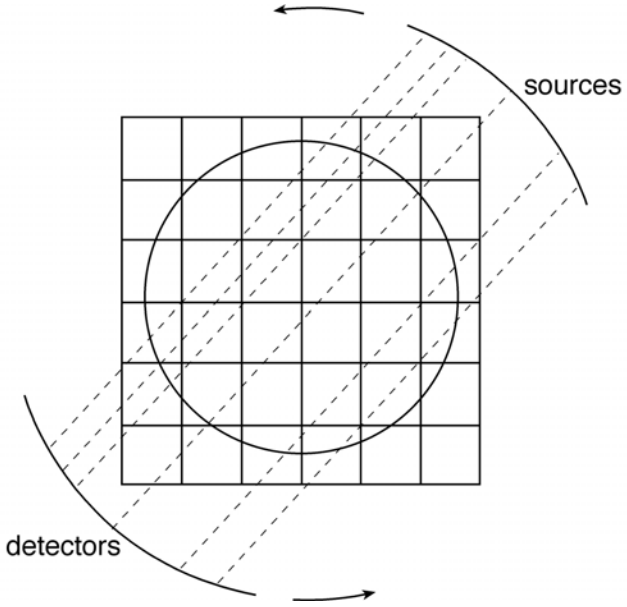

Figure 1.3: Generic tomographic problem in two dimensions. Measurements are made by integrating through an otherwise impenetrable solid between the transmitting sources and receivers using x-rays, sound, radio waves, etc. Properties can be anything measurable, including travel times, intensities, group velocities etc. The tomographic problem is to reconstruct the interior from these integrals. In the particular configuration shown, the source and receiver are supposed to revolve so that a very large number of paths can be built up. It is also supposed that the division into small rectangles is an adequate representation. In principle, one can have many more integrals than the number of squares defining the unknowns. {tomog1.tif}

A Tomographic Problem

So-called tomographic problems occur in many fields, most notably in medicine, but also in materials testing, oceanography, meteorology and geophysics. Generically, they arise when one is faced with the problem of inferring the distribution of properties inside an area or volume based upon a series of integrals through the region. Consider Fig. 1.3., where to be specific, suppose we are looking at the top of the head of a patient lying supine in a so-called CAT-scanner. The two external shell sectors represent in (a) a source of x-rays and, in (b) a set of x-ray detectors. X-rays are emitted from the source and travel through the patient along the indicated lines where the intensity of the received beam is measured. Let the absorptivity/unit length within the patient be a function, $c(\mathbf{r})$, where $\mathbf{r}$ is the vector position within the patient's head. Consider one source at $\mathbf{r}_s$ and a receptor at $\mathbf{r}_e$ connected by the path as indicated. Then the intensity measured at the receptor is,

$$I(\mathbf{r}_s, \mathbf{r}_r) = \int_{\mathbf{r}_s}^{\mathbf{r}_e} c(\mathbf{r}(s))\, ds, \tag{1.22}$$ {tomog1}

where s is the arc-length along the path. The basic tomographic problem is to determine $c(\mathbf{r})$ for all $\mathbf{r}$ in the patient, from measurements of I. In the medical problem, the shell sectors rotate around the patient, and an enormous number of integrals along (almost) all possible paths are obtained. An analytical solution to this problem, as the number of paths becomes infinite, is produced by the Radon transform.[4] Given that tumors and the like have a different absorptivity than does normal tissue, the reconstructed image of $c(\mathbf{r})$ permits physicians to "see" inside the patient. In most other situations, however, the number of paths tends to be much smaller than the formal number of unknowns and other solution methods must be found.

Note first, however, that we should modify Eq. (1.22) to reflect the inability of any system to produce a perfect measurement of the integral, and so more realistically we write,

$$I(\mathbf{r}_s, \mathbf{r}_r) = \int_{\mathbf{r}_s}^{\mathbf{r}_e} c(\mathbf{r}(s))\, ds + n(\mathbf{r}_s, \mathbf{r}_r), \tag{1.23}$$ {tomog2}

where n is the measurement noise.

To proceed, surround the patient with a bounding square (Fig. 1.4)—simply to produce a simple geometry—and divide the area into sub-squares as indicated, each numbered in sequence, $1 \leq j \leq N$. These squares are supposed sufficiently small that $c(\mathbf{r})$ is effectively constant within them. Also number the paths, $1 \leq i \leq M$. Then Eq. (1.23) can be approximated with arbitrary accuracy (by letting the sub-square dimensions become arbitrarily small) as,

$$I_i = \sum_{j=1}^{N} c_j \Delta r_{ij} + n_i. \tag{1.24}$$ {tomog3}

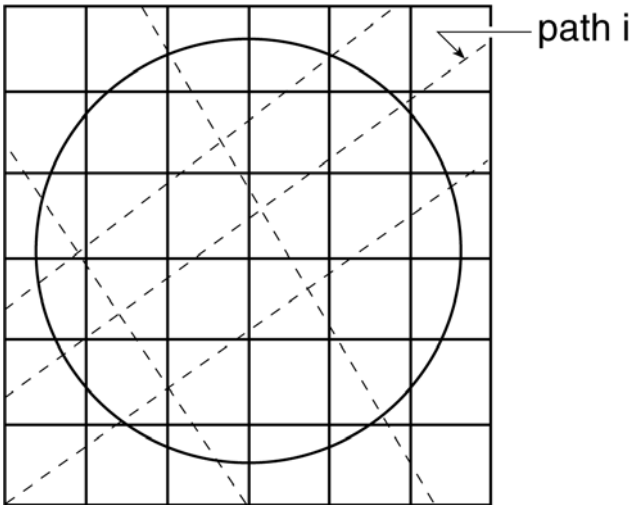

Figure 1.4: Simplified geometry for defining a tomographic problem. Some squares may have no integrals passing through them; others may be multiply-covered. Boxes outside the physical body can be handled in a number of ways, including the addition of constraints setting the corresponding $c_j = 0$. {tomog2.tif}

Here Δr_{ij} is the arc length of path i within square j (most of them will vanish for any particular path). Once again, these last equations are of the form

$$\mathbf{E}\mathbf{x} + \mathbf{n} = \mathbf{y}, \tag{1.25}$$ {canon1}

where here, $\mathbf{E} = \{\Delta r_{ij}\}$, $\mathbf{x} = [c_j]$, $\mathbf{n} = [n_i]$. Quite commonly there are many more unknown c_j than there are integrals I_i. (In the present context, there is no distinction between writing matrices $\mathbf{A}, \mathbf{E}$. $\mathbf{E}$ will generally be used where noise elements are present, and $\mathbf{A}$ where none are intended.)

Tomographic measurements do not always consist of x-ray intensities. In seismology or oceanography, for example, c_j is commonly $1/v_j$ where v_j is the speed of sound or seismic waves within the area; I is then a travel time rather than an intensity. The equations remain the same, however. This methodology also works in three-dimensions, the paths need not be straight lines and there are many generalizations.[5] A problem of great practical importance is determining what one can say about the solutions to Eqs. (4.34) even where many more unknowns exist than formal pieces of information y_i.

As with all these problems, many other forms of discretization are possible. For example,

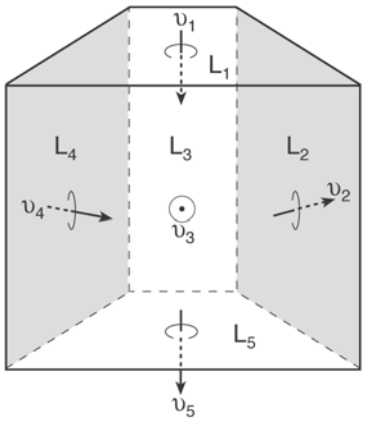

Figure 1.5: Volume of fluid bounded on four open sides across which fluid is supposed to flow. Mass is conserved, giving one relationship among the fluid transports v_i; conservation of one or more other tracers C_i leads to additional useful relationships. {track1.tif}

the continuous function $c(\mathbf{r})$ can be expanded,

$$c(\mathbf{r}) = \sum_q \sum_p a_{nm} T_n(r_x) T_m(r_y), \tag{1.26}$$

where $\mathbf{r} = (r_x, r_y)$, and the T_n are any suitable expansion functions (sines and cosines, Chebyschev polynomials, etc.). The linear equations (4.34) then represent constraints leading to the determination of the a_{nm}.

A Second Tracer Problem

Consider the closed volume in Fig. 1.5 enclosed by four boundaries as shown. There are steady flows, $v_i(z)$, $1 \leq i \leq 4$ either into or out of the volume, each carrying a corresponding fluid of constant density ρ_0. z is the vertical coordinate. If the width of each boundary is l_i, the statement that mass is conserved within the volume is simply,

$$\sum_{i=1}^{r} l_i \rho_0 \int_{-h}^{0} v_i(z)\, dz = 0, \tag{1.27}$$ {box1}

where the convention is made that flows into the box are positive, and flows out are negative. $z = -h$ is the lower boundary of the volume and $z = 0$ is the top one. If the v_i are unknown, Eq. (1.27) represents one equation (constraint) in four unknowns,

$$\int_{-h}^{0} v_i(z)\, dz, \ 1 \leq i \leq 4. \tag{1.28}$$

One possible, if boring, solution is $v_i(z) = 0$. To make the problem somewhat more interesting, we now suppose that for some mysterious reason, the vertical derivatives, $v_i'(z) = dv_i(z)/dz$,

are known so that,

$$v_i(z) = \int_{-z_o}^{z} v_i'(z)\,dz + b_i(z_0)\,, \tag{1.29}$$

where z_0 is a convenient place to start the integration (but can be any value). b_i are integration constants ($b_i = v_i(z_0)$) which remain unknown. Constraint (1.27) becomes,

$$\sum_{i=1}^{4} l_i \rho_0 \int_{-h}^{0} \left[\int_{-z_o}^{z} v_i'(z')\,dz' + b_i(z_0) \right] dz = 0, \tag{1.30}$$

or,

{box2}
$$\sum_{i=1}^{4} h l_i b_i(z_0) = -\sum_{i=1}^{4} l_i \int_{-h}^{0} dz \int_{-z_o}^{z} v_i'(z')\,dz' \tag{1.31}$$

where the right-hand side is known. Eq. (1.31) is still one equation in four unknown b_i, but the zero-solution is no longer possible, unless the right-hand side vanishes. Eq. (1.31) is a statement that the weighted average of the b_i on the left-hand-side is known. If one seeks to obtain estimates of the b_i separately, more information is required.

Suppose that information pertains to a tracer, perhaps a red-dye, known to be conservative, and that the box concentration of red-dye, C, is known to be in a steady-state. Then conservation of C becomes,

{box3}
$$\sum_{i=1}^{4} \left[h l_i \int_{-h}^{0} C_i(z)\,dz \right] b_i = -\sum_{i=1}^{4} l_i \int_{-h}^{0} dz \int_{-z_o}^{z} C_i(z')\, v_i'(z')\,dz', \tag{1.32}$$

where $C_i(z)$ is the concentration of red-dye on each boundary. Eq. (1.32) provides a second relationship for the four unknown b_i. One might try to measure another dye concentration, perhaps green dye, and write an equation for this second tracer, exactly analogous to (1.32). With enough such dye measurements, one might obtain more constraint equations than unknown b_i. In any case, no matter how many dyes are measured, the resulting equation set is of the form (1.9). The number of boundaries is not limited to four, but can be either fewer, or many more.[6]

Vibrating String

Consider a uniform vibrating string anchored at its ends $r_x = 0$, $r_x = L$. The free motion of the string is governed by the wave equation

$$\frac{\partial^2 \eta}{\partial r_x^2} - \frac{1}{c^2}\frac{\partial^2 \eta}{\partial t^2} = 0,\ c^2 = T/\rho, \tag{1.33}$$

where T is the tension, and ρ the density. Free modes of vibration (eigen-frequencies) are found to exist at discrete frequencies, s_q,

{vibrate2}
$$2\pi s_q = \frac{q\pi c}{L},\ q = 1, 2, 3, ..., \tag{1.34}$$

and which is the solution to a classical forward problem. A number of interesting and useful inverse problems can be formulated. For example, given $s_q \pm \Delta s_q$, $1 \leq q \leq M$, to determine L, or c. These are particularly simple problems, because there is only one parameter, either c or L to determine. More generally, it is obvious from Eq. (1.34) that one has information only about the ratio c/L—they could not be determined separately.

Suppose, however, that the density varies along the string, $\rho = \rho(r_x)$, so that $c = c(r_x)$. Then (it may be confirmed) that the observed frequencies are no longer given by Eq. (1.34), but by expressions involving the integral of c over the length of the string. An important problem is then to infer $c(r_x)$, and hence $\rho(r_x)$. One might wonder whether, under these new circumstances, L can be determined independently of c?

A host of such problems, in which the observed frequencies of free modes are used to infer properties of media in one to three dimensions exists. The most elaborate applications are in geophysics and solar physics, where the normal mode frequencies of the vibrating whole earth or sun are used to infer the interior properties for the earth (density and elastic parameters).[7] A good exercise is to render the spatially variable string problem in discrete form.

1.4 Importance of the Forward Model

Inference about the physical world from data requires assertions about the structure of the data and its internal relationships. One sometimes hears claims from people who are expert in measurements that "I don't use models." Such a claim is almost always vacuous. What the speaker usually means is that he doesn't use equations, but is manipulating his data in some simple way (e.g., forming an average) that seems to be so unsophisticated that no model is present. Consider, however, a simple problem faced by someone trying to determine the average temperature in a room. A thermometer is successively placed at different three-dimensional locations, $\mathbf{r}_i$, at times t_i. Let the measurements be y_i and the value of interest is,

$$\tilde{m} = \frac{1}{M}\sum_{i=1}^{M} y_i. \tag{1.35}$$ {mean1}

In deciding to compute, and use $\tilde{m}$, the observer has probably made a long list of very sophisticated, but implicit, model assumptions. Among them we might suggest: (1) Thermometers require assumptions about the quantity recorded (e.g., an oscillator frequency or a voltage) and the connection to the desired temperature as well as potentially elaborate calibration means. (2) That the temperature in the room is sufficiently slowly changing that all of the t_i can be regarded as effectively identical. A different observer might suggest that the temperature in the room is governed by shock waves bouncing between the walls at intervals of seconds or less.

Should that be true, $\tilde{m}$ constructed from the available samples might prove completely meaningless. It might be objected that such an hypothesis is far-fetched. But the assumption that the room temperature is governed, e.g., by a slowly evolving diffusion process, is a rigid, and perhaps incorrect model. (3) That the errors in the thermometer are such that the best estimate of the room mean temperature is obtained by the simple sum in Eq. (1.35). There are many measurement devices for which this assumption is a very poor one (perhaps the instrument is drifting, or has a calibration that varies with temperature), and we will discuss how to determine averages in Chapter 2. But the assumption that property $\tilde{m}$ is useful, is a strong model assumption concerning both the instrument being used and the physical process it is measuring.

This list can be extended (the interpretation of the mean is itself model-dependent), but more generally, the inverse problems listed earlier in this chapter only make sense to the degree that the underlying forward model is likely to be an adequate physical description of the observations. For example, if one is attempting to determine ρ in Eq. (1.15) by taking the Laplacian $\nabla^2\phi$, (analytically or numerically), this solution to the inverse problem is only sensible if this equation really represents the correct governing physics. If the correct equation to use were, instead,

$$\frac{\partial^2\phi}{\partial r_x^2} + \frac{1}{2}\frac{\partial\phi}{\partial r_y} = \rho, \tag{1.36}$$

where r_y is another coordinate, the calculated value of ρ would be incorrect. One might, however, have good reason to use Eq. (1.15) as the most likely hypothesis, but nonetheless remain open to the possibility that it is not an adequate descriptor of the required field, ρ. A good methodology, of the type we will develop in subsequent chapters, permits one to ask the question: is my model consistent with the data? If the answer to the question is "yes," a careful investigator would *never* claim that the resulting answer is the correct one and that the model has been "validated" or "verified." One claims only that the answer and the model are consistent with the observations, and remains open to the possibility that some new piece of information will be obtained that completely *invalidates* the model (e.g., some direct measurements of ρ showing that the inferred value is simply wrong). One can never validate or verify a model, one can only show consistency with existing observations.[8]

Notes

[1] See Lanczos (1961, Section 3.19)

[2] Whittaker and Robinson (1944)

[3] Lanczos (1961) has a much fuller discussion of this correspondence.

[4] Herman (1980).

[5] Herman (1980); Munk et al. (1995).

[6]Oceanographers will recognize this apparently highly artificicial problem as being a slightly simplified version of the so-called geostrophic inverse problem, and which is of great practical importance. It is a central subject in Chapter 5.

[7]Aki and Richards (1980). A famous two-dimensional version of the problem is described by Kac (1966); see also Gordon and Webb (1996).

[8]Oreskes et al. (1994).