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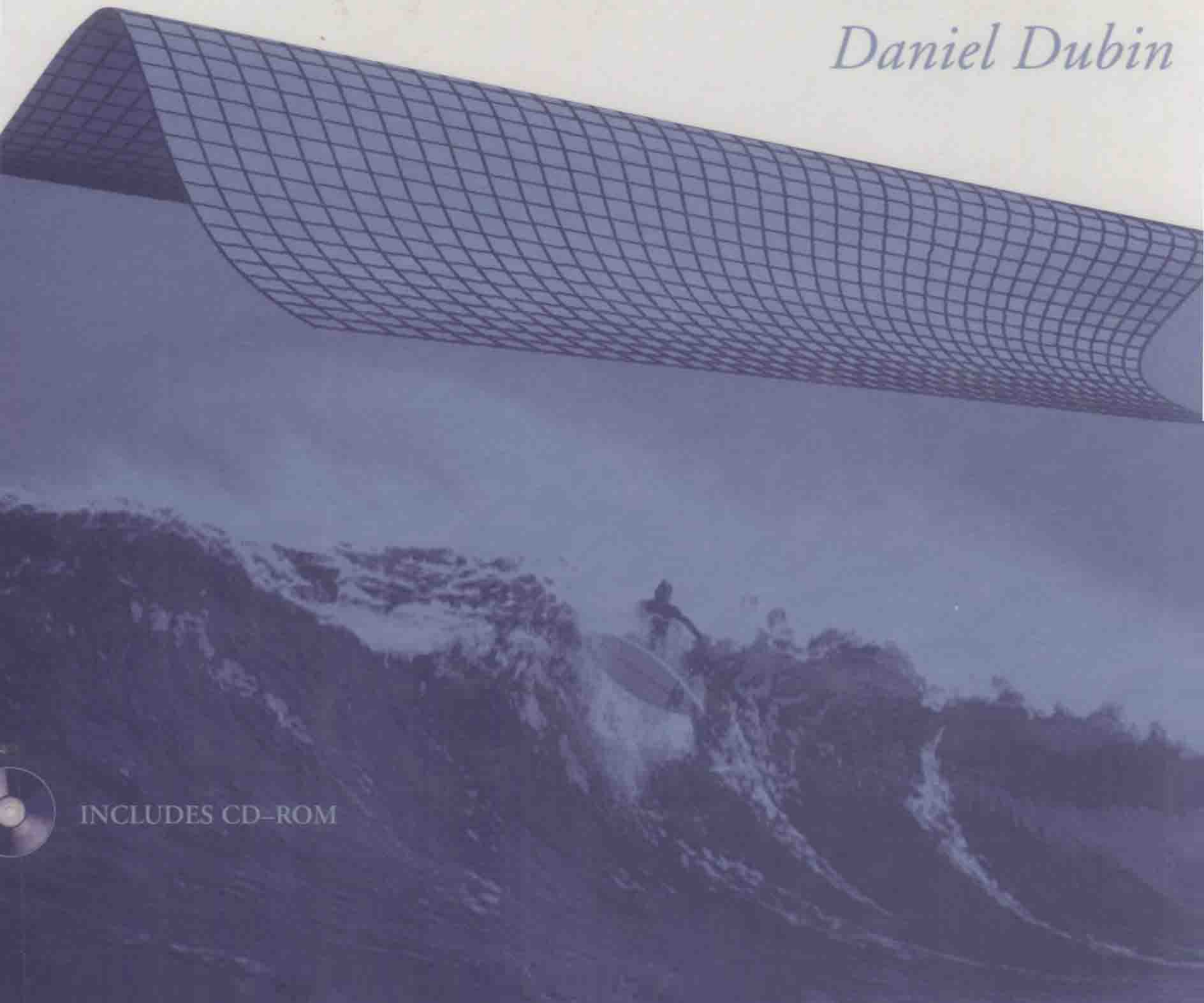
Numerical and Analytical Methods for Scientists and Engineers Using *Mathematica*®

Daniel Dubin



NUMERICAL AND ANALYTICAL METHODS FOR SCIENTISTS AND ENGINEERS USING *MATHEMATICA*

DANIEL DUBIN

WILEY-INTERSCIENCE

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UNIT CONVERSION

This book employs SI units. However, other units are sometimes preferable. Some conversion factors are listed below.

Length

1 Angstrom (Å) = 10^{-8} meter
1 foot = 0.305 meter
1 light year = 9.46×10^{15} meters
1 parsec = 3.26 light years

Volume

1 liter = 1000 centimeter^3 = 10^{-3} meter^3
1 U.S. gallon = 0.83 imperial gallon = 3.78 liters

Time

1 hour = 3600 seconds
1 day = 8.64×10^4 seconds
1 hertz (hz) = 1 second^{-1}

Mass

1 atomic mass unit (amu) = 1.6605×10^{-27} kilogram

Force

1 pound (lb) = 4.45 newtons

Energy and Power

1 erg = 10^{-7} joule
1 kcal = 1 Cal = 1000 cal = 4.184×10^3 joules
1 electron volt (eV) = 1.602×10^{-19} joule
1 foot-pound = 1.36 joules
1 horsepower = 746 watts

Pressure

1 atmosphere = 1.013 bar = 1.013×10^5 newtons/meter^2 = 14.7 pounds/inch^2 = 760 torr
1 pascal = 1 newton/meter^2

Temperature

x°C = $(273.16 + x)$K
x°F = $5(x - 32)/9$°C
1 eV = $k_B \times 11{,}605$ K

NUMERICAL AND ANALYTICAL METHODS FOR SCIENTISTS AND ENGINEERS USING *MATHEMATICA*

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PREFACE

TO THE STUDENT

Up to this point in your career you have been asked to use mathematics to solve rather elementary problems in the physical sciences. However, when you graduate and become a working scientist or engineer you will often be confronted with complex real-world problems. Understanding the material in this book is a first step toward developing the mathematical tools that you will need to solve such problems.

Much of the work detailed in the following chapters requires standard pencil-and-paper (i.e., analytical) methods. These methods include solution techniques for the partial differential equations of mathematical physics such as Poisson's equation, the wave equation, and Schrödinger's equation, Fourier series and transforms, and elementary probability theory and statistical methods. These methods are taught from the standpoint of a working scientist, not a mathematician. This means that in many cases, important theorems will be stated, not proved (although the ideas behind the proofs will usually be discussed). Physical intuition will be called upon more often than mathematical rigor.

Mastery of analytical techniques has always been and probably always will be of fundamental importance to a student's scientific education. However, of increasing importance in today's world are numerical methods. The numerical methods taught in this book will allow you to solve problems that cannot be solved analytically, and will also allow you to inspect the solutions to your problems using plots, animations, and even sounds, gaining intuition that is sometimes difficult to extract from dry algebra.

In an attempt to present these numerical methods in the most straightforward manner possible, this book employs the software package *Mathematica*. There are many other computational environments that we could have used instead—for example, software packages such as *Matlab* or *Maple* have similar graphical and numerical capabilities to *Mathematica*. Once the principles of one such package are learned, it is relatively easy to master the other packages. I chose *Mathematica* for this book because, in my opinion, it is the most flexible and sophisticated of such packages.

Another approach to learning numerical methods might be to write your own programs from scratch, using a language such as C or Fortran. This is an excellent way to learn the elements of numerical analysis, and eventually in your scientific careers you will probably be required to program in one or another of these languages. However, *Mathematica* provides us with a computational environment where it is much easier to quickly learn the *ideas* behind the various numerical methods, without the additional baggage of learning an operating system, mathematical and graphical libraries, or the complexities of the computer language itself.

An important feature of *Mathematica* is its ability to perform *analytical* calculations, such as the analytical solution of linear and nonlinear equations, integrals and derivatives, and Fourier transforms. You will find that these features can help to free you from the tedium of performing complicated algebra by hand, just as your calculator has freed you from having to do long division.

However, as with everything else in life, using *Mathematica* presents us with certain trade-offs. For instance, in part because it has been developed to provide a straightforward interface to the user, *Mathematica* is not suited for truly large-scale computations such as large molecular dynamics simulations with 1000 particles or more, or inversions of 100,000-by-100,000 matrices, for example. Such applications require a stripped-down precompiled code, running on a mainframe computer. Nevertheless, for the sort of introductory numerical problems covered in this book, the speed of *Mathematica* on a PC platform is more than sufficient. Once these numerical techniques have been learned using *Mathematica*, it should be relatively easy to transfer your new skills to a mainframe computing environment.

I should note here that this limitation does not affect the usefulness of *Mathematica* in the solution of the sort of small to intermediate-scale problems that working scientists often confront from day to day. In my own experience, hardly a day goes by when I do not fire up *Mathematica* to evaluate an integral or plot a function. For more than a decade now I have found this program to be truly useful, and I hope and expect that you will as well. (No, I am not receiving any kickbacks from Stephen Wolfram!)

There is another limitation to *Mathematica*. You will find that although *Mathematica* knows a lot of tricks, it is still a dumb program in the sense that it requires precise input from the user. A missing bracket or semicolon often will result in long paroxysms of error statements and less often will result in a dangerous lack of error messages and a subsequent incorrect answer. It is still true for this (or for any other software) package that garbage in = garbage out. Science fiction movies involving intelligent computers aside, this aphorism will probably hold for the foreseeable future. This means that, at least at first, you will spend a good fraction of your time cursing the computer screen. My advice is to get used to it—this is a process that you will go through over and over again as you use computers in your career. I guarantee that you will find it very satisfying when, after a long debugging session, you finally get the output you wanted. Eventually, with practice, you will become *Mathematica* masters.

I developed this book from course notes for two junior-level classes in mathematical methods that I have taught at UCSD for several years. The book is oriented toward students in the physical sciences and in engineering, at either the advanced undergraduate (junior or senior) or graduate level. It assumes an understanding of introductory calculus and ordinary differential equations. Chapters 1–8 also require a basic working knowledge of *Mathematica*. Chapter 9, included only in electronic form on the CD that accompanies this book, presents an introduction to the software's capabilities. I recommend that *Mathematica* novices read this chapter first, and do the exercises.

Some of the material in the book is rather advanced, and will be of more interest to graduate students or professionals. This material can obviously be skipped when the book is used in an undergraduate course. In order to reduce printing costs, four advanced topics appear only in the electronic chapters on the CD: Section 5.3 on wave action; Section 6.3 on numerically determined eigenmodes; Section 7.3 on the particle-in-cell method; and Section 8.3 on the Rosenbluth–Teller–Metropolis Monte Carlo method. These extra sections are highlighted in red in the electronic version.

Aside from these differences, the text and equations in the electronic and printed versions are, *in theory*, identical. However, I take sole responsibility for any inadvertent discrepancies, as the good people at Wiley were not involved in typesetting the electronic textbook.

The electronic version of this book has several features that are not available in printed textbooks:

1. ***Hyperlinks.*** There are hyperlinks in the text that can be used to view material from the web. Also, when the text refers to an equation, the equation number itself is a hyperlink that will take you to that equation. Furthermore, all items in the index and contents are linked to the corresponding material in the book, (For these features to work properly, all chapters must be located in the same directory on your computer.) You can return to the original reference using the **`Go Back`** command, located in the main menu under **`Find`**.
2. ***Mathematica Code.*** Certain portions of the book are *Mathematica* calculations that you can use to graph functions, solve differential equations, etc. These calculations can be modified at the reader's pleasure, and run *in situ*.
3. ***Animations and Interactive 3D Renderings.*** Some of the displayed figures are interactive three-dimensional renderings of curves or surfaces, which can be viewed from different angles using the mouse. An example is Fig. 1.13, the strange attractor for the Lorenz system. Also, some of the other figures are actually animations. Creating animations and interactive 3D plots is covered in Sections 9.6.7 and 9.6.6, respectively.
4. ***Searchable text.*** Using the commands in the **`Find`** menu, you can search through the text for words or phrases.

Equations or text may sometimes be typeset in a font that is too small to be read easily at the current magnification. You can increase (or decrease) the magnification of the notebook under the **Format** entry of the main menu (choose **Magnification**), or by choosing a magnification setting from the small window at the bottom left side of the notebook.

A number of individuals made important contributions to this project: Professor Tom O'Neil, who originally suggested that the electronic version should be written in *Mathematica* notebook format; Professor C. Fred Driscoll, who invented some of the problems on sound and hearing; Jo Ann Christina, who helped with the proofreading and indexing; and Dr. Jay Albert, who actually waded through the entire manuscript, found many errors and typos, and helped clear up fuzzy thinking in several places. Finally, to the many students who have passed through my computational physics classes here at UCSD: You have been subjected to two experiments—a *Mathematica*-based course that combines analytical and computational methods; and a book that allows the reader to interactively explore variations in the examples. Although you were beset by many vicissitudes (crashing computers, balky code, debugging sessions stretching into the wee hours) your interest, energy, and good humor were unflagging (for the most part!) and a constant source of inspiration. Thank you.

DANIEL DUBIN

La Jolla, California
March, 2003

CHAPTER 1

ORDINARY DIFFERENTIAL EQUATIONS IN THE PHYSICAL SCIENCES

1.1 INTRODUCTION

1.1.1 Definitions

Differential Equations, Unknown Functions, and Initial Conditions Three centuries ago, the great British mathematician, scientist, and curmudgeon Sir Isaac Newton and the German mathematician Gottfried von Liebniz independently introduced the world to calculus, and in so doing ushered in the modern scientific era. It has since been established in countless experiments that natural phenomena of all kinds can be described, often in exquisite detail, by the solutions to *differential equations*.

Differential equations involve derivatives of an *unknown function* or functions, whose form we try to determine through solution of the equations. For example, consider the motion (in one dimension) of a point particle of mass m under the action of a prescribed time-dependent force $F(t)$. The particle's velocity $v(t)$ satisfies Newton's second law

$$m\frac{dv}{dt} = F(t). \tag{1.1.1}$$

This is a differential equation for the unknown function $v(t)$.

Equation (1.1.1) is probably the simplest differential equation that one can write down. It can be solved by applying the *fundamental theorem of calculus*: for any function $f(t)$ whose derivative exists and is integrable on the interval $[a, b]$,

$$\int_a^b \frac{df}{dt}\,dt = f(b) - f(a). \tag{1.1.2}$$

Integrating both sides of Eq. (1.1.1) from an initial time $t = 0$ to time t and using Eq. (1.1.2) yields

$$\int_0^t \frac{dv}{dt}\,dt = v(t) - v(0) = \frac{1}{m}\int_0^t F(t)\,dt. \tag{1.1.3}$$

Therefore, the solution of Eq. (1.1.1) for the velocity at time t is given by the integral over time of the force, a known function, and an *initial condition*, the velocity at time $t = 0$. This initial condition can be thought of mathematically as a constant of integration that appears when the integral is applied to Eq. (1.1.1). Physically, the requirement that we need to know the initial velocity in order to find the velocity at later times is intuitively obvious. However, it also implies that the differential equation (1.1.1) by itself is not enough to completely determine a solution for $v(t)$; the initial velocity must also be provided. This is a general feature of differential equations:

Extra conditions beyond the equation itself must be supplied in order to completely determine a solution of a differential equation.

If the initial condition is *not* known, so that $v(0)$ is an undetermined constant in Eq. (1.1.3), then we call Eq. (1.1.3) a *general solution* to the differential equation, because different choices of the undetermined constant allow the solution to satisfy different initial conditions.

As a second example of a differential equation, let's now assume that the force in Eq. (1.1.1) depends on the position $x(t)$ of the particle according to Hooke's law:

$$F(t) = -kx(t), \tag{1.1.4}$$

where k is a constant (the spring constant). Then, using the definition of velocity as the rate of change of position,

$$v = \frac{dx}{dt}. \tag{1.1.5}$$

Eq. (1.1.1) becomes a differential equation for the unknown function $x(t)$:

$$\frac{d^2x}{dt^2} = -\frac{k}{m}x(t). \tag{1.1.6}$$

This familiar differential equation, the *harmonic oscillator* equation, has a general solution in terms of the trigonometric functions $\sin x$ and $\cos x$, and *two* undetermined constants C_1 and C_2:

$$x(t) = C_1\cos(\omega_0 t) + C_2\sin(\omega_0 t), \tag{1.1.7}$$

where $\omega_0 = \sqrt{k/m}$ is the natural frequency of the oscillation. The two constants

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can be determined by two initial conditions, on the initial position and velocity:

$$x(0) = x_0, \qquad v(0) = v_0. \tag{1.1.8}$$

Since Eq. (1.1.7) implies that $x(0) = C_1$ and $x'(0) = v(0) = \omega_0 C_2$, the solution can be written directly in terms of the initial conditions as

$$x(t) = x_0 \cos(\omega_0 t) + \frac{v_0}{\omega_0} \sin(\omega_0 t). \tag{1.1.9}$$

We can easily verify that this solution satisfies the differential equation by substituting it into Eq. (1.1.6):

Cell 1.1

```
x[t_] = x0 Cos[ω0 t] + v0/ω0 Sin[ ω0 t];
Simplify[x"[t] == -ω0^2 x[t]]

True
```

We can also verify that the solution matches the initial conditions:

Cell 1.2

```
x[0]

x0
```

Cell 1.3

```
x'[0]

v0
```

Order of a Differential Equation The *order* of a differential equation is the order of the highest derivative of the unknown function that appears in the equation. Since only a first derivative of $v(t)$ appears in Eq. (1.1.1), the equation is a *first-order* differential equation for $v(t)$. On the other hand, Equation (1.1.6) is a *second-order* differential equation.

Note that the general solution (1.1.3) of the first-order equation (1.1.1) involved one undetermined constant, but for the second-order equation, *two* undetermined constants were required in Eq. (1.1.7). It's easy to see why this must be so—an Nth-order differential equation involves the Nth derivative of the unknown function. To determine this function one needs to integrate the equation N times, giving N constants of integration.

The number of undetermined constants that enter the general solution of an ordinary differential equation equals the order of the equation.

Partial Differential Equations This statement applies only to *ordinary* differential equations (ODEs), which are differential equations for which derivatives of the unknown function are taken with respect to only a single variable. However, this book will also consider *partial* differential equations (PDEs), which involve derivatives of the unknown functions with respect to *several* variables. One example of a PDE is Poisson's equation, relating the electrostatic potential $\phi(x, y, z)$ to the charge density $\rho(x, y, z)$ of a distribution of charges:

$$\nabla^2\phi(x, y, z) = -\frac{\rho(x, y, z)}{\epsilon_0}. \qquad (1.1.10)$$

Here ϵ_0 is a constant (the dielectric permittivity of free space, given by $\epsilon_0 = 8.85\ldots \times 10^{-12}$ F/m), and ∇^2 is the *Laplacian operator*,

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}. \qquad (1.1.11)$$

We will find that ∇^2 appears frequently in the equations of mathematical physics.

Like ODEs, PDEs must be supplemented with extra conditions in order to obtain a specific solution. However, the form of these conditions become more complex than for ODEs. In the case of Poisson's equation, *boundary conditions* must be specified over one or more surfaces that bound the volume within which the solution for $\phi(x, y, z)$ is determined.

A discussion of solutions to Poisson's equation and other PDEs of mathematical physics can be found in Chapter 3 and later chapters. For now we will confine ourselves to ODEs. Many of the techniques used to solve ODEs can also be applied to PDEs.

> An ODE involves derivatives of the unknown function with respect to only a single variable. A PDE involves derivatives of the unknown function with respect to more than one variable.

Initial-Value and Boundary-Value Problems Even if we limit discussion to ODEs, there is still an important distinction to be made, between *initial-value problems* and *boundary-value problems*. In initial-value problems, the unknown function is required in some time domain $t > 0$ and all conditions to specify the solution are given at *one* end of this domain, at $t = 0$. Equations (1.1.3) and (1.1.9) are solutions of initial-value problems.

However, in boundary-value problems, conditions that specify the solution are given at different times or places. Examples of boundary-value problems in ODEs may be found in Sec. 1.5. (Problems involving PDEs are often boundary-value problems; Poisson's equation (1.1.10) is an example. In Chapter 3 we will find that some PDEs involving both time and space derivatives are solved as both boundary- *and* initial-value problems.)

For now, we will stick to a discussion of ODE initial-value problems.

In initial-value problems, all conditions to specify a solution are given at one point in time or space, and are termed *initial conditions*. In boundary-value problems, the conditions are given at several points in time or space, and are termed *boundary conditions*. For ODEs, the boundary conditions are usually given at two points, between which the solution to the ODE must be determined.

EXERCISES FOR SEC. 1.1

(1) Is Eq. (1.1.1) still a differential equation if the velocity $v(t)$ is given and the force $F(t)$ is the unknown function?

(2) Determine by substitution whether the following functions satisfy the given differential equation, and if so, state whether the functions are a general solution to the equation:

(a) $\dfrac{d^2x}{dt^2}=x(t),\ x(t)=C_1\sinh t+C_2e^{-t}.$

(b) $\left(\dfrac{dx}{dt}\right)^2=x(t),\ x(t)=\frac{1}{4}(a^2+t^2)-\dfrac{at}{2}.$

(c) $\dfrac{d^4x}{dt^4}-3\dfrac{d^3x}{dt^3}-7\dfrac{d^2x}{dt^2}+15\dfrac{dx}{dt}+18x=12t^2,\quad x(t)=a\,e^{3t}\,t+b\,e^{-2t}+\dfrac{2t^2}{3}-\dfrac{10t}{9}+\dfrac{13}{9}.$

(3) Prove by substitution that the following functions are general solutions to the given differential equations, and find values for the undetermined constants in order to match the boundary or initial conditions. Plot the solutions:

(a) $\dfrac{dx}{dt}=5x(t)-3,\ x(0)=1;\ x(t)=Ce^{5t}+3/5.$

(b) $\dfrac{d^2x}{dt^2}+4\dfrac{dx}{dt}+4x(t)=0,\ x(0)=0,\ x'(1)=-3;\ x(t)=C_1e^{-2t}+C_2te^{-2t}.$

(c) $\dfrac{d^3x}{dt^3}+\dfrac{dx}{dt}=t,\quad x(0)=0,\quad x'(0)=1,\quad x''(\pi)=0;\quad x(t)=t^2/2+C_1\sin t+C_2\cos t+C_3.$

1.2 GRAPHICAL SOLUTION OF INITIAL-VALUE PROBLEMS

1.2.1 Direction Fields; Existence and Uniqueness of Solutions

In an initial-value problem, how do we know when the initial conditions specify a *unique* solution to an ODE? And how do we know that the solution will even exist? These fundamental questions are addressed by the following theorem:

Theorem 1.1 Consider a general initial-value problem involving an Nth-order ODE of the form

$$\frac{d^N x}{dt^N} = f\left(t, x, \frac{dx}{dt}, \frac{d^2 x}{dt^2}, \ldots, \frac{d^{N-1} x}{dt^{N-1}}\right) \tag{1.2.1}$$

for some function f. The ODE is supplemented by N initial conditions on x and its derivatives of order $N-1$ and lower:

$$x(0) = x_0, \qquad \frac{dx}{dt} = v_0, \qquad \frac{d^2 x}{dt^2} = a_0, \ldots, \qquad \frac{d^{N-1}}{dt^{N-1}} = u_0.$$

Then, if the derivative of f in each of its arguments is continuous over some domain encompassing this initial condition, the solution to this problem exists and is unique for some length of time around the initial time.

Now, we are not going to give the proof to this theorem. (See, for instance, Boyce and Diprima for an accessible discussion of the proof.) But trying to understand it qualitatively is useful. To do so, let's consider a simple example of Eq. (1.2.1): the first-order ODE

$$\frac{dv}{dt} = f(t, v). \tag{1.2.2}$$

This equation can be thought of as Newton's second law for motion in one dimension due to a force that depends on both velocity and time.

Let's consider a graphical depiction of Eq. (1.2.2) in the (t, v) plane. At every point (t, v), the function $f(t, v)$ specifies the slope dv/dt of the solution $v(t)$. An example of one such solution is given in Fig. 1.1. At each point along the curve, the slope dv/dt is determined through Eq. (1.2.2) by $f(t, v)$. This slope is, geometrically speaking, an infinitesimal vector that is tangent to the curve at each of its points. A schematic representation of three of these infinitesimal vectors is shown in the figure.

The components of these vectors are

$$(dt, dv) = dt\left(1, \frac{dv}{dt}\right) = dt(1, f(t, v)). \tag{1.2.3}$$

The vectors $dt(1, f(t, v))$ form a type of *vector field* (a set of vectors, each member of which is associated with a separate point in some spatial domain) called a *direction field*. This field specifies the *direction* of the solutions at all points in the

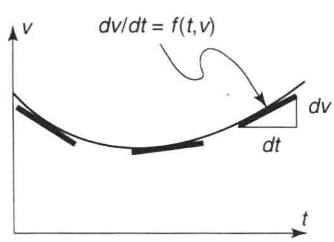

Fig. 1.1 A solution to $dv/dt = f(t, v)$.

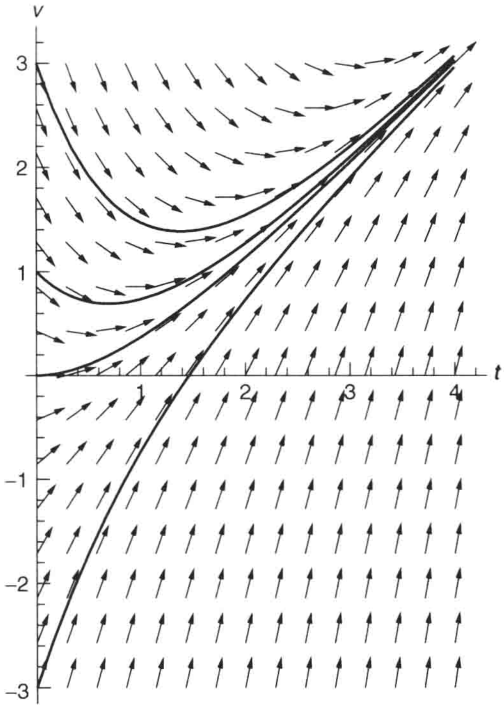

Fig. 1.2 Direction field for $dv/dt = t - v$, along with four solutions.

(t, v) plane: every solution to Eq. (1.2.2) for every initial condition must be a curve that runs tangent to the direction field. Individual vectors in the direction field are called *tangent vectors*.

By drawing these tangent vectors at a grid of points in the (t, v) plane (not infinitesimal vectors, of course; we will take dt to be finite so that we can see the vectors), we get an overall qualitative picture of solutions to the ODE. An example is shown in Figure 1.2. This direction field is drawn for the particular case of an acceleration given by

$$f(t, v) = t - v. \tag{1.2.4}$$

Along with the direction field, four solutions of Eq. (1.2.2) with different initial v's are shown. One can see that the direction field is tangent to each solution.

Figure 1.2 was created using a graphics function, available in *Mathematica*'s graphical add-on packages, that is made for plotting two-dimensional vector fields: **PlotVectorField**. The syntax for this function is given below:

```
PlotVectorField[{vx[x,y],vy[x,y]}, {x,xmin,xmax},{y,ymin,ymax},options].
```

The vector field in Fig. 1.2 was drawn with the following *Mathematica* commands:

Cell 1.4

```
<< Graphics`
```

Cell 1.5

```
f[t_, v_] = -v + t;
PlotVectorField[{1, f[t, v]}, {t, 0, 4}, {v, -3, 3},
Axes → True, ScaleFunction → (1 &), AxesLabel → {"t", "v"}]
```

The option **ScaleFunction->(1&)** makes all the vectors the same length. The plot shows that you don't really need the four superimposed solutions in order to see the qualitative behavior of solutions for different initial conditions—you can trace them by eye just by following the arrows.

However, for completeness we give the general solution of Eqs. (1.2.2) and (1.2.4) below:

$$v(t) = Ce^{-t} + t - 1, \tag{1.2.5}$$

which can be verified by substitution. In Fig. 1.2, the solutions traced out by the solid lines are for $C = [4, 2, 1 - 2]$. (These solutions were plotted with the **Plot** function and then superimposed on the vector field using the **Show** command.) One can see that for $t < \infty$, the different solutions never cross. Thus, specifying an initial condition leads to a *unique* solution of the differential equation. There are no places in the direction field where one sees convergence of two different solutions, except perhaps as $t \to \infty$. This is guaranteed by the differentiability of the function f in each of its arguments.

A simple example of what can happen when the function f is nondifferentiable at some point or points is given below. Consider the case

$$f(t, v) = v/t. \tag{1.2.6}$$

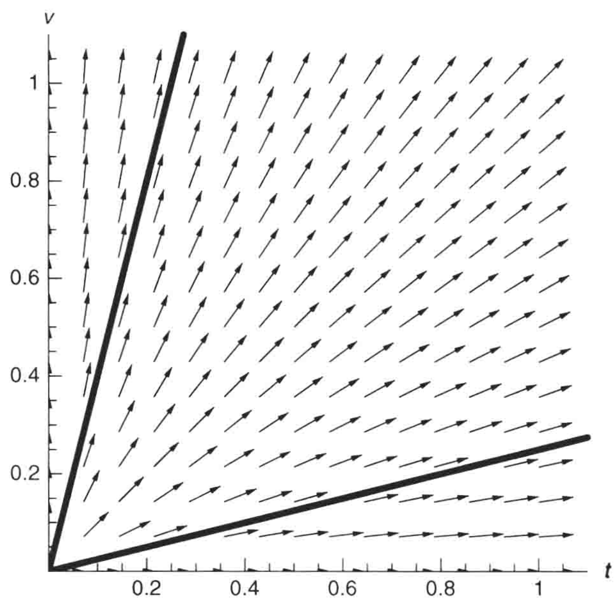

Fig. 1.3 Direction field for $dv/dt = v/t$, along with two solutions, both with initial condition $v(0) = 0$.

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