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Jeff Cash
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Solving Differential Equations in R

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To Carlo, Roslyn and Antonello

Preface

Mathematics plays an important role in many scientific and engineering disciplines. This book deals with the numerical solution of differential equations, a very important branch of mathematics. Our aim is to give a practical and theoretical account of how to solve a large variety of differential equations, comprising ordinary differential equations, initial value problems and boundary value problems, differential algebraic equations, partial differential equations and delay differential equations.

The solution of differential equations using R is the main focus of this book. It is therefore intended for the practitioner, the student and the scientist, who wants to know how to use R to solve differential equations.

When writing his famous book, "A Brief History of Time", Stephen Hawking [2] was told by his publisher that every equation he included in the book would cut its sales in half. When writing the current book, we have been mindful of this, and our main desire is to provide the reader with powerful numerical algorithms written in the R programming language for the solution of differential equations rather than considering the theory in any great detail.

However, we also bear in mind the famous statement of Kurt Lewin which is "there is nothing so practical as a good theory". Therefore each chapter that deals with R examples is preceded by a chapter where the theory behind the numerical methods being used is introduced. It has been our goal that non-mathematicians should at least understand the basics of the methods, while obtaining entrance into the relevant literature that provides more mathematical background. We believe that some knowledge of the fundamentals of the underlying algorithms is essential to use the software in an intelligent way, so the principles underlying the various methods should, at least at a basic level, be explained. Moreover, as this book is in the first place about R the discussion of the numerical methods will be skewed to what is actually available in R.

In the sections that deal with the use of R for solving differential equations, we have taken examples from a variety of disciplines, including biology, chemistry, physics, pharmacokinetics. Many are well-known test examples, used frequently in the field of numerical analysis.

R as a Problem Solving Environment

The choice of using R [8] may be surprising to people regularly involved in solving numerical problems. Powerful numerical methods for the solution of differential equations are typically programmed in e.g. Fortran, C, Java, or Python. Whereas these solution methods are often made freely available, it is unfortunately the case that one needs considerable programming expertise to be able to use them. In contrast, easy-to-use software is often in rather expensive programs, such as MATLAB, Maple or Mathematica. In line with this, most books that give practical information about how to solve differential equations make use of these big three problem solving environments, or of one of the free-of-charge variants.

Although still not often used for solving differential equations, R is also very well suited as a Problem Solving Environment. Apart from the fact that it is open source software, there are obvious advantages in solving differential equations in a software that is strong in visualisation and statistics. Moreover, more and more students are becoming acquainted with the language as its use in universities is growing rapidly, both for teaching and for research. This creates a unique opportunity to introduce these students to the powerful scientific methods which make use of differential equations.

The potential for using R to solve differential equations was initiated by the release of the R package **odesolve** by Woody Setzer, a biologist holding a bachelor's degree in mathematics from EPA, US [10]. Years later, a communication in the R-journal by Thomas Petzoldt, a biologist from the university of Dresden, Germany [5] showed the potential of R for solving initial value problems of ordinary differential equations in the field of ecology. Recently a number of books have applied R in the field of environmental modelling [12, 19]. Building upon this initial effort, Karline Soetaert, the first author of this book, (a biologist) in 2008 joined forces with Woody Setzer and Thomas Petzoldt to make an improved version of odesolve that was able to solve a much greater variety of differential equations. This resulted in the R package **deSolve** [17], which contains most of the integration methods available in R. Most of the solvers implemented in the R package **deSolve** are based on well-established numerical codes, programmed in Fortran. By using well tested, robust, reliable and powerful codes, more emphasis can be put on making the existing codes more versatile. For instance, most codes can now be used to solve delay differential equations, or to simulate events. Also, great care was taken to make a common interface that is (relatively) easy to apply from the user's point of view. A set of methods to solve partial differential equations by the method-of-lines was added to **deSolve**, while another package, **rootSolve** [11], was devised to efficiently solve partial differential equations and boundary value problems using root solving algorithms. Finally, solution methods for boundary value problems were implemented in R package **bvpSolve** [15], as a cooperation between the three authors from this book.

Because all these R packages share one common author (KS), there is a certain degree of consistency in them, which we hope to demonstrate here (see also [16]).

Quite a few other R packages deal with the implementation of differential equations [6, 13], with the solution of special types of differential equations [1, 3, 4, 7], with statistical analysis of their outputs [9, 14, 20], or provide test problems on which the various solvers can be benchmarked [18].

About the Three Authors

Mathematics is the playground not only for the mathematician and engineer who devise powerful mathematical techniques to solve particular classes of problems, but also for the scientist who applies these methods to real-world problems. Both disciplines meet at the level of software, the actual implementation of these methods in computer code.

The three authors reflect this duality and come from different disciplines. Jeff Cash and Francesca Mazzia are experts in numerical analysis in general and the construction of algorithms for solving differential equations in particular. In contrast Karline Soetaert is a biologist, with an additional degree in computer science, whose interest in these numerical methods is mainly due to the fact that she uses these algorithms for application in the field of the marine sciences. Although she originally wrote her scientific programs mainly in Fortran, since she came acquainted with R in 2007 she now performs nearly all of her scientific work in this programming environment.

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Chapter 1
Differential Equations

Abstract Differential equations (DEs) occur in many branches of science and technology, and there is a real need to solve them both accurately and efficiently. There are relatively few problems for which an analytic solution can be found, so if we want to solve a large class of problems, then we need to resort to numerical calculations. In this chapter we will give a very brief survey of the theory behind DEs and their solution. We introduce concepts such as analytic and numerical methods, the order of differential equations, existence and uniqueness of solutions, implicit and explicit methods. We end with a brief survey of the different types of differential equations that will be dealt with in later chapters of this book.

1.1 Basic Theory of Ordinary Differential Equations

Although the material contained in this section is largely of a theoretical nature it is presented at a rather basic level and the reader is advised to at least skim through it.

1.1.1 First Order Differential Equations

The general form taken by a first order ordinary differential equation (*ODE*) is

$$y' = f(x,y), \tag{1.1}$$

which may also be written as

$$\frac{dy}{dx} = f(x,y), \tag{1.2}$$

where f is a given function of x and y and y contained in $\Re^m$ is a vector. Here x is called the independent variable and $y = y(x)$ is the dependent variable.

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This equation is called *first order* as it contains no higher derivatives than the first. Furthermore, (1.1) is called an *ordinary* differential equation as y depends on one independent variable only.

1.1.2 Analytic and Numerical Solutions

A differentiable function $y(x)$ is a solution of (1.1) if for all x

$$y'(x) = f(x, y(x)). \tag{1.3}$$

If we suppose that $y(x_0)$ is known, the solution of (1.3), valid in the interval $[x_0, x_1]$, is obtained by integrating both sides of (1.1) with respect to x, to give:

$$y(x) - y(x_0) = \int_{x_0}^{x} f(t, y(t))dt, \quad x \in [x_0, x_1]. \tag{1.4}$$

In some cases this integral can be evaluated exactly to give an equation for y, and this is called an *analytic* solution. For example, the equation

$$y' = y^2 + 1, \tag{1.5}$$

has as analytic solution

$$y = \tan(x + c). \tag{1.6}$$

Note the free parameter c that occurs in the solution. It has been known for a long time that the solution of a first order equation contains a free parameter and that this solution is uniquely defined if for example we impose an initial condition of the form $y(x_0) = y_0$ and we suppose that the function f satisfies some regularity conditions. This is important and we will return to it later.

Unfortunately, it is true to say that many ordinary differential equations which appear to be quite harmless, in the sense that we could expect them to be easy to solve, cannot be solved analytically, i.e. the solution can not be expressed in terms of known functions. An illuminating example of this is given in [4, p. 4] where it is shown how "small changes" in the problem (1.5) may make it much harder (or impossible) to solve analytically. Indeed, if equation (1.5) is changed "slightly" to

$$y' = y^2 + x, \tag{1.7}$$

then the solution has a very complex structure in terms of Airy functions [4]. In view of this, and the fact that most "real-life" applications consist of complicated systems of equations, it is often necessary to approximate the solution by solving equation (1.1) *numerically* rather than analytically.

Undergraduate mathematics courses often give the impression that most differential equations can be solved analytically, with numerical techniques being developed to deal with those few classes of equations that have no analytic solution. In fact, the opposite is true: while an analytic solution is extremely useful if it does exist, experience shows that most equations of practical interest need to be solved numerically.

1.1.3 Higher Order Ordinary Differential Equations

In the previous section, we considered only the first order differential equation (1.1). Ordinary differential equations can include higher order derivatives as well. For example, second order equations of the form:

$$y'' = f(x, y, y'), \tag{1.8}$$

arise in many practical applications.

Normally, in order to deal with the second order equation (1.8), we first convert it to a system of first order equations. This we do by defining an extra dependent variable, which equals the first order derivative of y, in the following way:

$$\begin{aligned} y' &= y_1 \\ y_1' &= f(x, y, y_1). \end{aligned} \tag{1.9}$$

Rather than having one differential equation, we now have a system of two differential equations. Defining $Y = (y, y_1)^T$, (1.9) is of the form (1.1), with $Y \in \Re^2$. As we will see later (Sect. 1.1.4) we need to specify two conditions to define the solution uniquely in this second order case.

As a simple example consider a small stone falling through the air from a tower. Gravity produces an acceleration of $g = 9.8\ \mathrm{ms}^{-2}$, while the air exerts a resistive force which is proportional to the velocity (v). The differential equation describing this is:

$$v' = g - kv. \tag{1.10}$$

If we are interested in the distance from the top of the tower (x), we use the fact that the velocity $v = x'$, and the equation becomes a second order differential equation:

$$x'' = g - kx'. \tag{1.11}$$

Now, in order to solve (1.11), we rewrite it as two first order equations.

$$\begin{aligned} x' &= v \\ v' &= g - kv. \end{aligned} \tag{1.12}$$

This technique carries over to higher order equations as well. If we are faced with the numerical solution of an nth order equation, it is often advisable to first reduce