Two-Point Boundary Value Problems: Shooting Methods

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PREFACE

Two-point boundary value problems associated with systems of linear and nonlinear ordinary differential equations occur in many branches of mathematics, engineering, and the various sciences. In these problems, conditions are specified at the endpoints of an interval, and a solution of the differential equations over the interval is sought which satisfies the given endpoint conditions. Generally the equations cannot be solved analytically, so recourse must be made to a numerical approach. In this book we describe, develop, and exploit one such class of methods; namely, shooting methods. In a shooting method, a set of values of the unspecified conditions at the initial point of the interval ("missing initial conditions") is assumed, and the differential equations are numerically integrated to the terminal point ("shooting" at the target terminal points). If the computed terminal values satisfy the specified terminal conditions, the problem has been solved. If they do not (the normal course of events), the differences between the computed and specified terminal conditions (the "miss distances") are used to adjust the missing initial conditions. If the differential equations and boundary conditions are linear, the adjustment need only be made once, but if the differential equations or the boundary conditions are nonlinear, the adjustment of the missing initial conditions is an iterative process.

In the past, shooting methods were regarded with a certain amount of suspicion, chiefly for two reasons. The first had to do with the lack of a theoretical foundation for the iterative process just described, with the result that conditions under which the iterative process converged and estimates of the rate of convergence were not available. The second reason concerns the apparent inability of shooting methods to handle numerically sensitive (unstable) problems.

We first became aware of the lack of an adequate theory when we tried to reconcile some anomalous results produced by the Goodman-Lance method of adjoints, one of the best known and widely used shooting methods. Once we discovered that the Goodman-Lance procedure was a concrete realization of the abstract Newton-Kantorovich method, we had in hand a satisfactory theory of convergence and error estimates for it, and, subsequently, for other shooting methods as well. Then we were able to devise extensions of shooting methods, such as continuation, which enabled them to handle numerically sensitive problems. In this book we develop the basic methods and their extensions, along with the appropriate theory, and illustrate the techniques by applying them to a variety of problems drawn from practice.

Our book is intended for applied mathematicians and engineers, students and professionals, who are familiar with the numerical integration of initial value problems, and who want to solve two-point boundary value problems with a minimum of problem preparation. Since we believe that computing is the art of the possible, we give the methods in sufficient detail that the reader can generate his own programs. A well designed shooting method program will be independent of the particular problem to be solved, with the exception of the subroutine into which the right hand side of the set of ordinary differential equations to be solved is inserted. Our methods work just as well on small machines as on large ones.

While our main concern is to produce working tools for the applied mathematician and engineer, we do not think that these tools can be used properly without an understanding of the underlying theory. We have chosen to develop the necessary theory in the framework of functional analysis, following Kantorovich (who first exploited the application of functional analysis to applied mathematics and numerical analysis), Collatz, and others. We have found that functional analysis unifies seemingly disparate results, and that it often furnishes valuable geometrical insight through which a known procedure can be better understood, and new techniques developed.

Since we realize that many of our readers may not be acquainted with the concepts and terminology of functional analysis we have attempted throughout the text to restate key phrases and ideas in more familiar terms. In addition, we have included an Appendix in which the various concepts and terms are defined rigorously. Occupying, as we do, the middle ground between the mathematician and the engineer, we hope our stance of generating and explaining practical methods with sufficient theoretical underpinning will bridge the gap between their disciplines.

While our emphasis is on shooting methods, we also devote space to other methods, in particular, quasilinearization and finite difference methods, which have wide applicability in the computer solution of two-point boundary value problems. We regret not having been able to include still other approaches (invariant imbedding, for example), but we believe that the methods in this book will give the analyst a repertoire of techniques which should enable him to solve numerically the majority of two-point boundary value problems he is likely to encounter. This, in fact, has been our experience for we ourselves have solved almost every one of the numerical examples presented in this text by at least one, and often several, of the methods discussed.

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Chapter 1

INTRODUCTION

The purpose of this book is to describe in some detail various "shooting" and related methods for the numerical solution of two-point boundary value problems for linear and nonlinear ordinary differential equations. Two-point boundary value problems occur in a number of areas of applied mathematics, theoretical physics, and engineering, among them boundary layer theory, the study of stellar interiors, and control and optimization theory. Since it is usually impossible to obtain analytic (closed-form) solutions to the two-point boundary value problems met in practice, these problems must be attacked by numerical methods. The methods treated in this book have enabled applied mathematicians, programmers, and engineers who are not specialists in two-point boundary value problems to obtain numerical solutions to a wide variety of problems, within the time limits so often placed on their work.

In contrast to initial value problems for ordinary differential equations in which all the conditions are specified for one value of the independent variable (the initial point), two-point boundary value problems, as the name implies, have the property that conditions are specified at two values of the independent variable (the initial point and the final point; collectively, the boundary points). *

This apparently minor change can lead to profound changes in the behavior of the solution of the differential equations. It is not hard to give examples of linear differential equations that possess unique solutions as initial value problems, but which may have no solution, a unique solution, or an infinite number of solutions as two-point boundary value problems. For example, the initial value problem

$$\ddot{y}+y = 0, \qquad y(0) = c_1, \qquad \dot{y}(0) = c_2$$

has the unique solution $y(x) = c_1 \cos x + c_2 \sin x$ for any set of values c_1, c_2.

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* Multipoint boundary value problems, in which data are specified at more than two values of the independent variable, are sometimes encountered. Methods for handling such problems are not treated at length, but it is pointed out how certain of the methods can be generalized to handle multipoint boundary value problems.

However, the boundary value problem

$$\ddot{y}+y = 0, \qquad y(0) = 1, \qquad y(\pi) = 0$$

has no solution; the problem

$$\ddot{y}+y = 0, \qquad y(0) = 1, \qquad y(2) = 0$$

has the unique solution $y(x) = \cos x - (\text{cotan } 2) \sin x$; while the problem

$$\ddot{y}+y = 0, \qquad y(0) = 0, \qquad y(\pi) = 0$$

has an infinite number of solutions $y(x) = B \sin x$, where B may have any value.

In the examples above, values of the solution at the two ends of the interval were specified, and different combinations of end points and values of the solution led to different conditions of existence and uniqueness of solutions. The specification of the derivative of the solution, rather than the value of the solution itself, may also lead to different conclusions with regard to the existence and uniqueness of solutions of two-point boundary value problems. Consider, for example, the differential equation

$$\ddot{y}+f(y, \dot{y}, x) = 0,$$

where $f(y, \dot{y}, x)$ is continuous in the strip D: $-\infty \leqq y \leqq \infty$, $-\infty \leqq \dot{y} \leqq \infty$, $a \leqq x \leqq b$, and $f(y, \dot{y}, x)$, satisfies the Lipschitz condition

$$|f(y, \dot{y}, x) - f(u, \dot{u}, x)| \leqq K|y-u| + L|\dot{y}-\dot{u}|,$$

where K and L are positive constants and y, $\dot{y}$, u, $\dot{u}$ are points in D. Then Bailey *et al.* [1] show that the existence of a unique solution to the two-point boundary value problem $y(a) = A$, $y(b) = B$ can be guaranteed over an interval $[a, b]$ *twice as long* as the interval for which existence and uniqueness obtain for the problem $y(a) = A$, $\dot{y}(b) = m$.

In view of the complicated behavior that solutions of two-point boundary value problems can exhibit, it should not be surprising that the theory of the existence and uniqueness of solutions of these problems is in a less satisfactory condition than the corresponding theory for initial value problems. And it should be expected that the numerical solution of a two-point boundary problem for a given ordinary differential equation will in general be a more difficult matter than the numerical solution of the corresponding initial value problem.

There now exist a number of efficient methods for the step-by-step numerical integration of initial value problems, and it is assumed that the reader is familiar with the use of standard one-step methods such as Runge-Kutta and multistep methods such as Hamming's modification of Milne's method.

These methods have in common that the solution is computed at a succession of values of the independent variable, say $x_1, x_2, x_3, \ldots$, where x_0 is the initial point. The initial conditions at x_0 contain sufficient information for the solution to be computed at x_1; and so on. (The progression of the solution from x_0 to x_1 to x_2, etc., explains why initial value problems are sometimes called "marching" problems.) Iteration at the points x_i is sometimes used to improve the numerical accuracy, but no "guessing" is involved because the method has already furnished a good first approximation. In two-point boundary value problems, on the other hand, there is not sufficient information at the initial point to start a step-by-step solution; hence a way must be found to determine the missing initial conditions, or an approach other than step-by-step integration must be used. Also, iteration is more likely to be an essential feature of a method for the solution of two-point boundary value problems, and it is usual that missing initial conditions or even solution profiles must be guessed, with no other *a priori* knowledge.

Two-point boundary value problems have been attacked by a variety of techniques, among them:

1. Interpolation methods. Solutions of the differential equations are found by numerical integration for sets of values of the missing initial conditions. These solutions will not in general satisfy the prescribed boundary conditions. The correct values of the missing initial conditions are then found by inverse interpolation [2, 3].

2. Variational methods. The two-point boundary value problem is replaced by the variational problem of minimizing a certain integral, and the resulting variational problem is solved by the Rayleigh-Ritz methods [2, 4].

3. Method of collocation. The solution of the two-point boundary value problem is represented by a function of several parameters which satisfies the boundary conditions for any set of values of the parameters. The approximate solution is substituted in the differential equations and the parameters are determined by the satisfaction of some error criterion [2].

4. Picard's method. The two-point boundary value problem is put in a form symbolically represented by $x = F(x)$. A sequence of approximate solutions $x^{(n)}$ is developed by the process $x^{(n)} = F(x^{(n-1)})$ which converges to the solution of the original problem under certain conditions [1–3].

5. Discrete methods. The derivatives occurring in the differential equations are replaced by appropriate finite differences, and the solution to the two-point boundary value is sought at discrete values of the independent variable. The effect is to replace the original problem by the problem of solving a finite number of algebraic or transcendental equations [2–6].

6. Quasilinearization. In this method, applicable only to two-point boundary value problems for systems of nonlinear ordinary differential equations, the original nonlinear problem is replaced by a sequence of more easily solved linear problems whose solutions converge under appropriate conditions to the solution of the original problem [7, 8].

7. Shooting methods. They take their name from the situation in the two-point boundary value problem for a single second-order differential equation with initial and final values of the solution prescribed. Varying the initial slope gives rise to a set of profiles which suggest the trajectory of a projectile "shot" from the initial point. That initial slope is sought which results in the trajectory "hitting" the target; that is, the final value [1, 6, 8–11].

This hit-or-miss method is of course unsuitable for the solution of two-point boundary value problems on high-speed digital computers. What is needed is a systematic way to vary the missing conditions based on the amount by which the final values are missed. The shooting methods we are concerned with have this property. In fact, linear problems can be solved by shooting methods without iteration, and the iterations necessary for nonlinear problems can be shown to converge under appropriate conditions.

For nonlinear differential equations, shooting methods have certain advantages for the problem solver. First of all, the methods are quite general and are applicable to a wide variety of differential equations. It is not necessary for the applicability of shooting methods that the equations be of special types such as even-order self-adjoint. Second, shooting methods require a minimum of problem analysis and preparation. It is relatively easy to implement shooting methods on digital computers using standard subroutines for the numerical integration of ordinary differential equations, solutions of linear algebraic equations, etc. With a properly written code, only one subroutine need be altered from problem to problem, the one in which the right-hand side of the system of differential equations written in a standard form is entered. All other parts of the code will handle automatically any problem from a broad class.

Despite their advantages, shooting methods, like all methods, have their limitations. Shooting methods sometimes fail to converge for problems which are sensitive to the initial conditions. In some problems modest changes in the initial conditions result in numerical difficulties such as machine overflow. Procedures such as continuation and reorthogonalization have been developed which extend the usefulness of shooting methods, and they are discussed.

However, problems are sometimes encountered in practice which cannot be solved even by the extended shooting methods. For this reason we have included a brief treatment of finite difference methods, one of whose virtues is their capability of handling numerically sensitive problems. We also discuss quasilinearization, which has been successfully applied to the practical solution of two-point boundary value problems.

Several apparently different shooting methods have been presented in the literature, often as purely formal manipulations with little attention to the conditions under which the methods work. Our emphasis here is on the derivation of the various methods, their interrelationships, and the demonstration that they are all realizations of a generalization of the familiar Newton-Raphson method for the solution of equations. Once the shooting methods are shown to be a kind of Newton-Raphson method, conditions for convergence, rates of convergence, and error estimates can be derived. In addition, we are concerned with the practical computer implementation of the techniques, and the solution of problems that arise in scientific and engineering applications.

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Chapter 2

SHOOTING METHODS

2.1. INTRODUCTION

In this chapter we discuss the statement of the two-point boundary value problems as dealt with in this book; namely, in terms of a system of first-order ordinary differential equations. The reduction of higher-order systems of differential equations to a system of first-order differential equations is described. A brief description of each of the shooting methods is given.

2.2. TWO-POINT BOUNDARY VALUE PROBLEM STATEMENT

Two point-boundary value problems are problems in which, for a set of possibly nonlinear ordinary differential equations, some boundary conditions are specified at the initial value of the independent variable, while the remainder of the boundary conditions are specified at the terminal value of the independent variable. The boundary conditions are therefore split between the two points, the initial and terminal values of the independent variable.

In this book, by two-point boundary value problems we mean problems with the following characteristics:

1. n first-order ordinary differential equations to be solved over the interval $[t_0, t_f]$, where t is the independent variable, t_0 is the initial point, and t_f is the final point.

2. r boundary conditions specified at the initial value of the independent variable.

3. $(n - r)$ boundary conditions specified at the terminal value of the independent variable.

As a rule, the differential equations will be nonlinear, but linear equations will play an important role in the numerical methods to be developed.

Problems originally expressed as higher-order nonlinear ordinary differential equations can be reduced to a system of first-order nonlinear ordinary differential equations as described in Section 2.3.

In this book the two-point boundary value problem is written as follows: The set of n nonlinear ordinary differential equations is

$$\dot{y}_i = g_i(y_1, y_2, \ldots, y_n, t), \qquad i = 1, 2, \ldots, n, \tag{2.2.1}$$

where the differential equations can be explicitly solved for the derivative, the g_i functions are assumed to be twice differentiable with respect to each of the dependent variables y_j, t is the independent variable, and $\dot{y}_i = dy_i/dt$.

The initial boundary conditions at the initial independent variable t_0 are

$$y_i(t_0) = c_i, \qquad i = 1, 2, \ldots, r. \tag{2.2.2}$$

The terminal boundary conditions at the terminal value of the independent variable t_f are

$$y_{i_m}(t_f) = c_{i_m}, \qquad m = 1, 2, \ldots, n-r. \tag{2.2.3}$$

More complicated boundary conditions can be given, but they usually can be reduced to the statement above or can be handled with modest changes in the shooting procedures. See Chapter 3, Section 3.8. Moreover, problems are sometimes encountered in which conditions are specified at more than two points (multipoint boundary value problems), but they are not treated here at length. See Chapter 8, Sections 8.7 and 8.8.

This statement of the problem assumes that the equations and variables can be renamed or reordered so the first r variables will have boundary conditions specified at the initial independent variable.

The subscripts on the specified terminal conditions are written i_m to allow for the possibility that the set of variables specified at the initial value of the independent variable and the set of variables specified at the final value of the independent variable may not be disjoint. For example, let the number of equations $n = 6$; let the initial boundary conditions be specified for $y_1(t_0), y_2(t_0)$, and $y_3(t_0)$; and let the terminal conditions be given for $y_2(t_f), y_4(t_f)$, and $y_6(t_f)$. Under these circumstances, y_2 is fixed at both the initial and final points; therefore the sets of variables specified at the initial and terminal points are not disjoint. Note that y_5 is not given at either the initial or terminal points. The indexing for the terminal conditions is therefore $i_1 = 2$, $i_2 = 4$, $i_3 = 6$, so $y_{i_1}(t_f)$ is $y_2(t_f)$, $y_{i_2}(t_f)$ is $y_4(t_f)$, and $y_{i_3}(t_f)$ is $y_6(t_f)$.

It should be mentioned here that the indexing for both the initial and terminal conditions is a convenient device to state the two-point boundary value problem concisely for purposes of discussion. In practice we do not rename or reorder the equations every time the boundary conditions are changed. For a computer solution of the two-point boundary value problem, we indicate in the input data to the program which variables are specified at the initial and final values of the independent variable and which variables are not specified. The computer program then tests each variable against the input data and treats each variable accordingly. Thus the "bookkeeping" of the variables specified at the initial and terminal values of the independent variable is handled automatically by the code.

2.3. REDUCTION OF *n*th-ORDER EQUATION

It is convenient to reduce all higher-order differential equations to a system of first-order equations. From an analysis point of view and from a computer program point of view, we can then focus our attention on essentially one class of problem.

The method for doing this is standard: Given a single *n*th-order nonlinear ordinary differential equation

$$y^{(n)}(t) = g(y, y^{(1)}, y^{(2)}, \ldots, y^{(n-1)}, t),$$

where

$$y^{(k)} = \frac{d^k y}{dt^k},$$

we define a system of n first-order nonlinear differential equations as follows:

$$\begin{aligned} y_1 &= y, \\ y_2 &= \dot{y}_1 = y^{(1)}, \\ y_3 &= \dot{y}_2 = \ddot{y}_1 = y^{(2)}, \\ &\vdots \\ y_n &= \dot{y}_{n-1} = \ldots = y^{(n-1)}, \end{aligned}$$

where

$$\dot{y}_k = dy_k/dt.$$

The $y^{(n)}(t)$ equation is therefore replaced by the system of n first-order nonlinear ordinary differential equations

$$\begin{aligned} \dot{y}_n &= g(y_1, y_2, \ldots, y_n, t), \\ \dot{y}_{n-1} &= y_n, \\ \dot{y}_{n-2} &= y_{n-1}, \\ &\vdots \\ \dot{y}_1 &= y_2. \end{aligned}$$

Thus any system of higher-order ordinary differential equations can be reduced to a system of first-order ordinary differential equations.

2.4. ANALYTICAL SOLUTION

If the differential equation can be solved analytically, then the two-point boundary value problem can generally be solved without difficulty. For linear differential equations the solution of a two-point boundary value problem reduces to determining the values of the constants from the given boundary conditions as the solution to a set of linear algebraic equations.

Consider the following example which, because of the simplicity of the problem, we do not bother to put in the form (2.2.1):

$$\frac{d^2y}{dt^2} = y+t, \qquad y(0) = 0, \qquad y(1) = 1.$$

The solution of the homogeneous differential equations is

$$y_h(t) = c_1 e^t + c_2 e^{-t},$$

while the particular solution is

$$y_p(t) = -t.$$

The general solution is therefore

$$y(t) = y_h(t) + y_p(t) = c_1 e^t + c_2 e^{-t} - t.$$

By the first boundary condition,

$$y(0) = 0 = c_1 + c_2$$

and, by the second boundary condition,

$$y(1) = 1 = c_1 e + c_2 e^{-1} - 1.$$

Solving this set of linear algebraic equations for c_1 and c_2 gives

$$c_1 = -c_2 = \frac{2}{e-e^{-1}} = \frac{1}{\sinh 1}.$$

The general solution is therefore

$$y(t) = \frac{2\sinh t}{\sinh 1} - t.$$