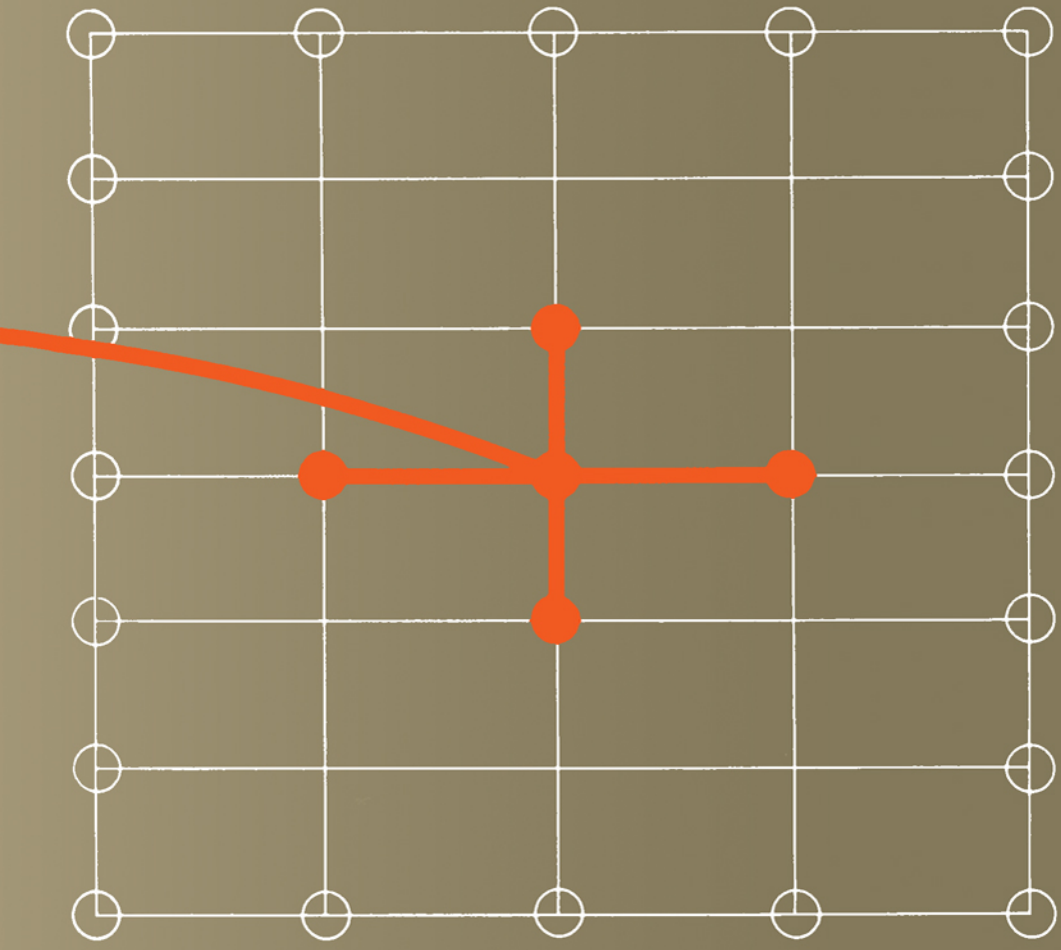
THE NUMERICAL SOLUTION OF ORDINARY AND PARTIAL DIFFERENTIAL EQUATIONS

Granville Sewell



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GRANVILLE SEWELL

Mathematics Department
University of Texas at El Paso
El Paso, Texas

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In memory of my father,

Edward G. Sewell (1919–1987)

who made us understand the words: "whoever would be great among you must be your servant."

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Preface

The roots of this text can be traced back to a short syllabus entitled "Solución Numérica de Ecuaciones Diferenciales," written in 1974 for a course at Universidad Simon Bolivar in Caracas. It is still a short book to have as wide a scope as implied by the title, but we believe it gives a solid introduction to the computer solution of ordinary and partial differential equations, appropriate for a senior level undergraduate or first year graduate course.

The student taking a course based on this text should have had introductory courses in multivariate calculus, linear algebra, and general numerical analysis. A formal course in ordinary or partial differential equations would be useful but is not essential, provided the student has been exposed to such equations in applications or in the numerical analysis course.

After a review of direct methods for the solution of linear systems in Chapter 0, with emphasis on the special features of the linear systems that arise when differential equations are solved, the following four chapters introduce and analyze the more commonly used finite difference methods for solving a variety of problems, including both ordinary differential equations (ODEs) and partial differential equations (PDEs), and both initial value and

boundary value problems. The techniques studied in these chapters are quite easy to implement, and after finishing Chapter 4 the student should be able to solve a wide range of differential equations. The finite difference methods used to solve partial differential equations in Chapters 2–4 are mostly classical low order formulas, easy to program but not ideal for problems with poorly behaved solutions or (especially) for problems in irregular multi-dimensional regions. More complicated finite difference techniques are not studied in this text. It is our philosophy that finite difference methods are still useful only because they are easy to program and to understand. When these methods become complex (e.g., when problems with irregular domains are solved), they cease to be attractive, and finite element methods should be used.

Chapter 5 contains an overview of the basic ideas behind the finite element method. After finishing this chapter, the student should have a good idea of what the finite element method is all about, and should even be able to use it to solve many simple problems. However, the student who wants to be able to write programs that efficiently solve more difficult problems should continue his/her study using the text *Analysis of a Finite Element Method: PDE/PROTRAN*, by Granville Sewell [Springer-Verlag, 1985]. This is a reference book for PDE/PROTRAN, IMSL's partial differential equation package (see Section 5.6), but it can be used as a supplementary text for a course in the numerical solution of differential equations. Chapter 5 provides an excellent introduction for the PDE/PROTRAN text, since it examines many of the ideas discussed in that book in a simpler, less general, context. The PDE/PROTRAN book can be considered as a companion text for this one, and a course that covers both would provide a good practical and theoretical understanding of the numerical solution of differential equations.

An important feature of the current text is that FORTRAN77 programs are given that implement many of the methods studied, and the reader can see how these techniques are implemented efficiently. Machine-readable copies of the FORTRAN77 programs displayed in this book are available upon request from the author.

0

Direct Solution of Linear Systems

0.0 Introduction

The problem of solving a system of N simultaneous linear equations in N unknowns arises frequently in the study of the numerical solution of differential equations: when an implicit method is used to solve an initial value problem, and when almost any method is used to solve a boundary value problem. Direct methods to solve such systems are based on Gaussian elimination, a process whose basic ideas should be familiar to the student. However, those systems that arise during the numerical solution of differential equations tend to have certain characteristics that can be exploited using appropriate variations to the basic elimination algorithm. In this chapter we review Gaussian elimination and look at some of these special characteristics.

0.1 General Linear Systems

The basic idea behind Gaussian elimination is to reduce the linear system $A\mathbf{x} = \mathbf{b}$ to an equivalent triangular system by interchanging rows (equations) and adding a multiple of one row (equation) to another. Then the equations

of the reduced (triangular) system are solved in reverse order, by back substitution. The reduction is done systematically, zeroing all the subdiagonal elements in the first column, then those below α_{22}, etc., until all subdiagonal elements are zero and the system is triangular. To zero the subdiagonal element $\alpha_{ik}(i > k)$, we add $-\alpha_{ik}/\alpha_{kk}$ times the kth row to the ith row (Figure 0.1.1) and add the same multiple of b_k to b_i. If α_{kk} (called the

$$\begin{array}{cccccc|c} \times & \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times & \times \\ 0 & 0 & \alpha_{kk} & \times & \times & \times & b_k \\ 0 & 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \alpha_{ik} & \times & \times & \times & b_i \\ 0 & 0 & \times & \times & \times & \times & \times \end{array}$$

Figure 0.1.1

"pivot") is zero, of course, we must switch row k with another row that contains a nonzero element in the kth column. We do not want to switch with a row above the kth row, because that would cause some of the elements in previous columns to become nonzero again, after they have been zeroed. Thus we must select one of the elements $\alpha_{kk}, \alpha_{k+1,k}, \ldots, \alpha_{Nk}$ as the next pivot and bring it to the pivot position by switching its row with the kth row. If all of these potential pivots are also zero, the matrix is singular, and we must give up. To see this, notice that in this case the last $N - k + 1$ rows of A each contain nonzero elements only in the last $N - k$ columns. These rows must be linearly dependent, because a maximum of $N - k$ independent rows can exist in an $N - k$ dimensional space. Since Gaussian elimination does not alter the rank of a matrix, the original matrix must have had dependent rows, and therefore it must have been singular.

On the other hand, if the potential pivots are not all zero, we face the question of which to use. If pivoting is only done when $\alpha_{kk} = 0$, this can lead to bad numerical results, for a nearly zero pivot is almost as bad as a zero one, as the following example illustrates.

Consider the two by two linear system

$$\begin{bmatrix} \varepsilon & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1 + \varepsilon \\ 2 \end{bmatrix},$$

which has (1, 1) as its exact solution. If ε is very small, this system is *not* ill-conditioned (nearly singular). Its determinant is $\varepsilon - 1$, or almost -1. Yet