NUMERICAL ANALYSIS FOR APPLIED MATHEMATICS, SCIENCE, AND ENGINEERING

Donald Greenspan • Vincenzo Casulli

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Donald Greenspan
University of Texas at Arlington

and

Vincenzo Casulli
University of Trento, Italy

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PREFACE

This book is designed for a first course in numerical analysis. It differs considerably from other such texts in its choice of topics. Our concern has been with the needs of science, engineering and applied mathematics students, who, in increasing numbers, form a majority of the students in numerical analysis courses. Thus, we have presented a broad spectrum of topics of applied interest, which, in fact, bring the reader to various frontiers of the subject. We have been able to do this by purging the traditional curriculum of many topics which are not likely to be encountered in either science or technology. These topics include, for example, number systems, computer operations, the secant method, Weddle's rule, Richardson extrapolation, and the methods of Graeffe and Milne. Related decisions were guided by a desire to include nonlinear equations, in addition to linear ones.

The need to solve a wide spectrum of nonlinear problems has been increasing since the end of the nineteenth century. For example, accurate simulation of dynamical processes related to planetary motion, rocket propulsion, turbulent flow, chemical oscillators, diffusion processes, and elastic stress demand the ability to solve nonlinear equations. Accurate fitting of data derived by use of laser technology, atomic clocks, electron microscopes and/or radio telescopes requires greater sophistication than that available from a linear least square fit. Quantitative methodology applicable to large classes of nonlinear problems became available only with the development of modern digital computers, and the result has been, and probably will continue to be, an explosion of knowledge.

In the final chapter, we have included a study of the Navier-Stokes equations, a fully nonlinear system of fluid dynamical equations which, interestingly enough, can be derived from both the macro, or hydrodynamic, approach and a micro, or molecular, approach. These equations are among the most challenging in contemporary numerical analysis and are fundamental to diverse studies relating to such areas as weather prediction, aerodynamics, petroleum recovery, cardiovascular circulation, heat convection, ocean currents, and the not-so-ordinary flow of ordinary water in pipes. Interest in the Navier-Stokes equations is so broad that we felt their inclusion to be appropriate.

One of the major goals in writing this book was to develop methodology for which the numerical solution of a given problem has the same qualitative behavior as the analytical solution, for, thereby, the numerical solution preserves the physics of a given mathematical model. Another major goal was to develop numerical analysis in such a fashion that the reader would be able to apply the methods thoughtfully and within a reasonably short time to problems which he or she finds both interesting and significant. For this reason, methodology, theory and intuition have been interwoven throughout.

The book is suitable for a junior, senior or first year graduate course. Only a familiarity with computer programming and ordinary differential equations is assumed throughout. We have set stars before various sections to denote material of relative difficulty. Chapters 1-5, exclusive of the starred sections, provide ample material for a one semester undergraduate course, assuming computer implementation by the student. In their entirety, these chapters can be used for a one semester graduate course. Chapters 6-9 are designed for the second half of a full year course. These chapters deal with partial differential equations, and, in each, the first few sections develop the necessary mathematical background. Note that a star has been affixed to the title of Chapter 9 to indicate the advanced nature of the entire chapter. Observe also that the exercises have been divided into two sets, basic ones and supplementary ones. Among the supplementary ones are several unexpected surprises.

In our own teaching, our philosophy has been that computer implementation by the student is essential. As a consequence, the time required for the study of various topics has been greater than that required in a purely theoretical lecture course. Nevertheless, from an applied point of view, a numerical algorithm that does not run on a computer is useless, and the student should verify an algorithm's viability by direct computer implementation. Theory is important in numerical analysis, but theory, alone, will fail to meet the needs of the majority of our students.

Finally, we wish to thank those undergraduate students at the University of Trento and those undergraduate and graduate students at the University of Texas at Arlington who contributed in so many ways to the final structure of the book. Unfortunately, the list of names is too long for inclusion.

D. Greenspan
V. Casulli
1988

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1

Algebraic and Transcendental Systems

1.1 INTRODUCTION

Science is study of Nature. We study Nature not only because we are curious, but because we would like to control its very powerful forces. Understanding the ways in which Nature works might enable us to grow more food, to prevent normal cells from becoming cancerous, and to develop relatively inexpensive sources of energy. In cases where control may not be possible, we would like to be able to predict what will happen. Thus, being able to predict when and where an earthquake will strike might save many lives, even though, at present, we have no expectation of being able to prevent a quake itself.

The discovery of knowledge by scientific means is carried out in the following way. First, there are experimental scientists who, as meticulously as possible, reach conclusions from experiments and observations. Since no one is perfect, not even a scientist, all experimental conclusions have some degree of error. Hopefully, the error will be small. Then, there are the theoretical scientists, who create models from which conclusions are reached, often using mathematical methods. Experimental scientists are constantly checking these models by planning and carrying out new experiments. Theoreticians are constantly refining their models by incorporating new experimental results. The two groups work in a constant check-and-balance refinement process to create knowledge. And only after extensive experimental verification and widespread professional agreement is a scientific conclusion accepted as valid.

Scientific experimentation and observation require mathematical methodology for handling and analyzing data sets. Scientific modeling requires mathematical methodology for solving equations and systems of equations. In this book we will develop basic, constructive techniques for both these areas of endeavor. And, though the development will be relatively elementary, we will, throughout, use the exceptional arithmetic power available through the application of modern, high-speed digital computers. The resulting methods are called numerical methods.

It is natural, then, since the arithmetical operations performed by modern computers are those of classical algebra, that we begin with the study of algebraic and transcendental systems of equations.

1.2 Matrices and Linear Systems

For $n \geq 2$, the general linear algebraic system of n equations in the n unknowns $x_1, x_2, x_3, \ldots, x_n$ can be written in the form

$$
\begin{aligned}
&a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n = b_1 \\
&a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots + a_{2n}x_n = b_2 \\
&a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \ldots + a_{3n}x_n = b_3 \\
&\quad \vdots \qquad \vdots \qquad \vdots \qquad\qquad \vdots \qquad \vdots \\
&a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \ldots + a_{nn}x_n = b_n \,.
\end{aligned}
\tag{1.1}
$$

If matrix **A** and vectors **x** and **b** are defined by

$$
\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{bmatrix}, \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix},
\tag{1.2}
$$

then system (1.1) can be written compactly as

$$
\mathbf{A}\,\mathbf{x} = \mathbf{b} \,.
\tag{1.3}
$$

Of course, forms (1.1) and (1.3) are equivalent. For ***theoretical*** discussions, however, (1.3) will be the more convenient one.

Unless otherwise stated, it should be noted that, throughout, we will concern ourselves only with real numbers and real functions.

From a computer point of view, it is desirable to know that system (1.1) has ***one and only one*** solution before one attempts to solve it. Numerical computations for systems which have more than one solution usually yield meaningless results. Numerical computations for systems which have no solutions are always meaningless. The fundamental theorem which assures such existence and uniqueness and is proved in introductory algebra courses is stated now for completeness.

THEOREM 1.1. System (1.1) has one and only one solution if and only if the determinant of A, denoted by |A|, is different from zero.

Theoretically, when $|A|\neq 0$, the solution of (1.1) for given **A** and **b** can be given constructively as the quotient of determinants by Cramer's rule. For example, for system

$$
\begin{aligned}
x_1+x_2-x_3 &= 2\\
x_1-x_2+x_3 &= 0\\
-x_1+x_2+x_3 &= 0\,,
\end{aligned}
$$

one has, by Cramer's rule,

$$
x_1=\frac{\begin{vmatrix} 2 & 1 & -1\\ 0 & -1 & 1\\ 0 & 1 & 1\end{vmatrix}}{\begin{vmatrix} 1 & 1 & -1\\ 1 & -1 & 1\\ -1 & 1 & 1\end{vmatrix}},\qquad
x_2=\frac{\begin{vmatrix} 1 & 2 & -1\\ 1 & 0 & 1\\ -1 & 0 & 1\end{vmatrix}}{\begin{vmatrix} 1 & 1 & -1\\ 1 & -1 & 1\\ -1 & 1 & 1\end{vmatrix}},\qquad
x_3=\frac{\begin{vmatrix} 1 & 1 & 2\\ 1 & -1 & 0\\ -1 & 1 & 0\end{vmatrix}}{\begin{vmatrix} 1 & 1 & -1\\ 1 & -1 & 1\\ -1 & 1 & 1\end{vmatrix}},
$$

so that

$$x_1=1\,,\qquad x_2=1\,,\qquad x_3=0\,.$$

Cramer's rule, however, though reasonable for n=2,3 and 4, becomes readily intractable for increasing values of n because the determinants are difficult to evaluate, and other methods must be used. Since we will be interested often in relatively large values of n, let us introduce next some matrix properties which are common in many applied problems and which will enable us to solve (1.1) quickly and efficiently. In general, the more structure which is imposed on **A**, the easier it will be to solve (1.1). One must be sure, however, when studying an applied problem, that the structure which has been imposed is consistent with the physical constraints of the problem.

DEFINITION 1.1. System (1.1) is said to be *diagonally dominant* if and only if

$$(1.4)\qquad |a_{ii}| \geq \sum_{\substack{j=1\\ j\neq i}}^{n} |a_{ij}|\,,\qquad i=1,2,\ldots,n,$$

with strict inequality valid for at least one value of i.

EXAMPLE 1. The following system is diagonally dominant:

$$\begin{aligned} -4x_1+2x_2+x_3+x_4 &= 2\\ -x_1-5x_2+x_3+x_4 &= -1\\ 3x_1+x_2-6x_3+2x_4 &= 0\\ x_1+x_2+2x_3-4x_4 &= -1\,. \end{aligned}$$

EXAMPLE 2. The following system is not diagonally dominant, but interchange of the second and third equations yields a system which is:

$$\begin{aligned} -4x_1+2x_2+x_3+x_4 &= 2\\ 3x_1+x_2-6x_3+2x_4 &= 0\\ -x_1-5x_2+x_3+x_4 &= -1\\ x_1+x_2+2x_3-4x_4 &= -1\,. \end{aligned}$$

EXAMPLE 3. The following system is not diagonally dominant, nor is any system which results by reordering the equations:

$$\begin{aligned} -x_1+x_2+x_3+x_4 &= -1\\ x_1-x_2+x_3+x_4 &= -1\\ x_1+x_2-x_3+x_4 &= -1\\ x_1+x_2+x_3-x_4 &= -1\,. \end{aligned}$$

DEFINITION 1.2. System (1.1) is said to be *tridiagonal* if and only if all elements of A are zero except a_{ii}, $a_{j,j+1}$, $a_{j+1,j}$, $i=1,2,\ldots,n$; $j=1,2,\ldots,n-1$, and none of these is zero.

EXAMPLE. The following system is tridiagonal:

$$\begin{aligned} -3x_1+x_2 &= 1\\ x_1-2x_2+x_3 &= -1\\ x_2-2x_3+x_4 &= 11\\ x_3-2x_4+x_5 &= 2\\ x_4-2x_5 &= -3\,. \end{aligned}$$

The term tridiagonal, in the last definition, is most appropriate because, in matrix form, **A** has the particular representation

$$A = \begin{bmatrix} a_{11} & a_{12} & & & & & 0 \\ a_{21} & a_{22} & a_{23} & & & & \\ & a_{32} & a_{33} & a_{34} & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & \cdot \\ & 0 & & & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \\ & & & & & a_{n,n-1} & a_{n,n} \end{bmatrix},$$

in which all elements are zero except those on three diagonals: the main diagonal, the superdiagonal (just above the main diagonal), and the subdiagonal (just below the main diagonal).

We turn now to practical methods of solution.

1.3 GAUSS ELIMINATION

If one knows only that $|A| \neq 0$, it may be difficult to solve (1.1) for large n. The method often applied first is an elementary one called Gauss elimination, which is reviewed next by means of an example.

Consider the system

$$4x_1 - x_2 + 2x_3 - x_4 = 2 \tag{1.5}$$

$$x_1 + 4x_2 - x_3 + x_4 = 2 \tag{1.6}$$

$$x_1 - 2x_2 - 3x_3 + x_4 = 4 \tag{1.7}$$

$$x_2 - 4x_4 = 0\,. \tag{1.8}$$

It is verified easily that the determinant of the system has the value 290, so that the solution exists and is unique. Next, we add suitable multiples of (1.5) to (1.6), (1.7) and (1.8) to eliminate x_1 in these equations. In this way (1.6)-(1.8) reduce to

$$\frac{17}{4}x_2 - \frac{3}{2}x_3 + \frac{5}{4}x_4 = \frac{3}{2} \tag{1.6'}$$

$$-\frac{7}{4}x_2 - \frac{7}{2}x_3 + \frac{5}{4}x_4 = \frac{7}{2} \tag{1.7'}$$

$$x_2 \qquad - 4x_4 = 0\,. \tag{1.8'}$$

Next, add suitable multiples of (1.6') to each of (1.7') and (1.8') to eliminate x_2 in these equations. In this way, (1.7') and (1.8') reduce to

$$-\frac{70}{17}x_3 + \frac{30}{17}x_4 = \frac{70}{17} \tag{1.7''}$$

$$\frac{6}{17}x_3 - \frac{73}{17}x_4 = -\frac{6}{17}\,. \tag{1.8''}$$

Next, add a suitable multiple of (1.7") to (1.8") to eliminate x_3 in (1.8"). In this way, (1.8") reduces to

$$-\frac{29}{7}x_4 = 0\,. \tag{1.8'''}$$

Thus, system (1.5)-(1.8) has been transformed into the equivalent system

$$4x_1 - x_2 + 2x_3 \quad - x_4 = 2 \tag{1.5}$$

$$\frac{17}{4}x_2 - \frac{3}{2}x_3 + \frac{5}{4}x_4 = \frac{3}{2} \tag{1.6'}$$

$$-\frac{70}{17}x_3 + \frac{30}{17}x_4 = \frac{70}{17} \tag{1.7''}$$

$$-\frac{29}{7}x_4 = 0\,. \tag{1.8'''}$$

Finally, the latter system is solved by backward substitution, that is, from (1.8"') one has $x_4=0$; substitution of $x_4=0$ into (1.7") yields $x_3=-1$; substitution of $x_4=0$ and $x_3=-1$ into (1.6') yields $x_2=0$; and substitution of $x_4=0$, $x_3=-1$, $x_2=0$ into (1.5) yields $x_1=1$, and the original system is solved.

With a little thought and a few self-generated examples, one can see readily how to direct a digital computer to perform Gauss elimination. The mathematical recipe, or set of mathematical directions, to do this is a particular example of what is called formally an ***algorithm.*** To develop a Gauss elimination algorithm, one must formalize the ***elimination*** and the ***backward*** substitution steps, which are the basic elements of the method. Now, with regard to the elimination step, we must have a means to indicate how the element a_{ij} in the i-th row and j-th column changes during the process. This is accomplished by using the symbol $a_{ij}^{(k)}$, where k is a positive integer and will indicate that the original a_{ij} has been adjusted (k–1) times. With these abbreviations and notations in mind, we next observe that the elimination step can be stated very precisely as follows. Set $a_{ij}^{(1)}=a_{ij}$, $b_i^{(1)}=b_i$. Then, for k=1,2,...,n–1, generate $a_{ij}^{(k+1)}$ and $b_i^{(k+1)}$ recursively by

$$(1.9) \qquad a_{ij}^{(k+1)} = a_{ij}^{(k)} - \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}} a_{kj}^{(k)}, \qquad b_i^{(k+1)} = b_i^{(k)} - \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}} b_k^{(k)},$$

for i,j=k+1,k+2,...,n–1,n. The system one then has is

$$\begin{aligned}
a_{11}^{(1)}x_1+a_{12}^{(1)}x_2+a_{13}^{(1)}x_3+ \dots +a_{1n}^{(1)}x_n &= b_1^{(1)}\\
a_{22}^{(2)}x_2+a_{23}^{(2)}x_3+ \dots +a_{2n}^{(2)}x_n &= b_2^{(2)}\\
a_{33}^{(3)}x_3+ \dots +a_{3n}^{(3)}x_n &= b_3^{(3)}\\
\vdots \qquad \vdots \qquad &\vdots\\
a_{nn}^{(n)}x_n &= b_n^{(n)}.
\end{aligned}$$

Finally, the backward substitution step is

$$(1.10) \qquad x_n = \frac{b_n^{(n)}}{a_{nn}^{(n)}}, \qquad x_i = \frac{b_i^{(i)} - \sum_{j=i+1}^{n} a_{ij}^{(i)}x_j}{a_{ii}^{(i)}}, \qquad i=n-1,n-2,\dots,2,1,$$

and the algorithm is complete.

In Gauss elimination, if any of the elements $a_{kk}^{(k)}$, which are called the ***pivot*** elements, vanishes or, in absolute value, becomes very small compared to the other elements $a_{ik}^{(k)}$, i>k, then we attempt to rearrange the remaining rows so as to attain a nonvanishing pivot or to avoid multiplication by a large number. Specifically, for each k we choose j, the smallest integer for which $|a_{jk}^{(k)}|=\max_{i>k}|a_{ik}^{(k)}|$ and interchange rows k and j. This strategy is called ***pivoting***. If A is diagonally dominant then no pivoting is necessary.

EXAMPLE. Consider the system

$$x_2 - 4x_4 = 0 \tag{1.11}$$

$$x_1 - 2x_2 - 3x_3 + x_4 = 4 \tag{1.12}$$

$$x_1 + 4x_2 - x_3 + x_4 = 2 \tag{1.13}$$

$$4x_1 - x_2 + 2x_3 - x_4 = 2\,. \tag{1.14}$$

In this case, since $a_{11}^{(1)}=0$, there is no multiple of (1.11) which can be added to (1.12), (1.13) and (1.14) to eliminate x_1 in these equations. However, since $|a_{41}^{(1)}|=\max|a_{i1}^{(1)}|$, interchange of equations (1.11) and (1.14) leads to the following equivalent system

$$4x_1 - x_2 + 2x_3 - x_4 = 2 \tag{1.14}$$

$$x_1 - 2x_2 - 3x_3 + x_4 = 4 \tag{1.12}$$

$$x_1 + 4x_2 - x_3 + x_4 = 2 \tag{1.13}$$

$$x_2 - 4x_4 = 0\,. \tag{1.11}$$

Now, for k=1, use of (1.9) yields

$$-\frac{7}{4}x_2 - \frac{7}{2}x_3 + \frac{5}{4}x_4 = \frac{7}{2} \tag{1.12'}$$

$$\frac{17}{4}x_2 - \frac{3}{2}x_3 + \frac{5}{4}x_4 = \frac{3}{2} \tag{1.13'}$$

$$x_2 - 4x_4 = 0\,. \tag{1.11'}$$

Next, since the pivot element $a_{22}^{(2)}=-\frac{7}{4}$ in (1.12') is smaller in absolute value than $a_{32}^{(2)}=-\frac{17}{4}$, we interchange (1.12') with (1.13'):

$$\frac{17}{4}x_2 - \frac{3}{2}x_3 + \frac{5}{4}x_4 = \frac{3}{2} \tag{1.13'}$$

$$-\frac{7}{4}x_2 - \frac{7}{2}x_3 + \frac{5}{4}x_4 = \frac{7}{2} \tag{1.12'}$$

$$x_2 - 4x_4 = 0 \tag{1.11'}$$