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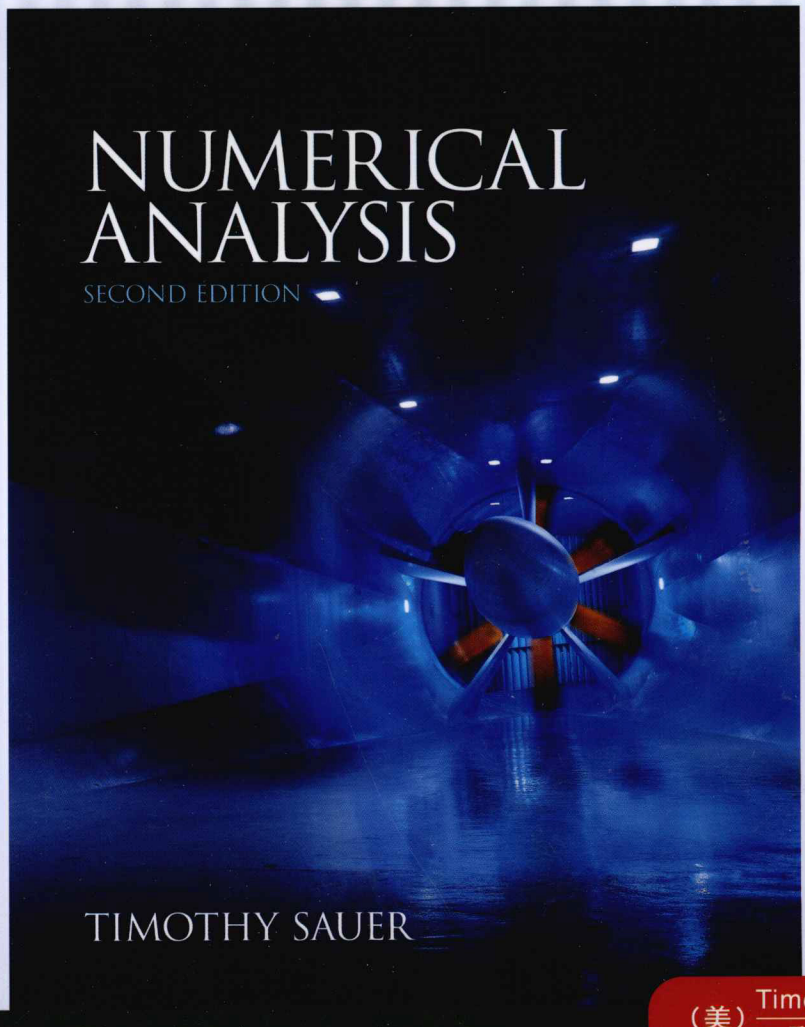

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机械工业出版社
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Numerical Analysis

(Second Edition)

（美）Timothy Sauer 著
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Preface

Numerical Analysis is a text for students of engineering, science, mathematics, and computer science who have completed elementary calculus and matrix algebra. The primary goal is to construct and explore algorithms for solving science and engineering problems. The not-so-secret secondary mission is to help the reader locate these algorithms in a landscape of some potent and far-reaching principles. These unifying principles, taken together, constitute a dynamic field of current research and development in modern numerical and computational science.

The discipline of numerical analysis is jam-packed with useful ideas. Textbooks run the risk of presenting the subject as a bag of neat but unrelated tricks. For a deep understanding, readers need to learn much more than how to code Newton's Method, Runge–Kutta, and the Fast Fourier Transform. They must absorb the big principles, the ones that permeate numerical analysis and integrate its competing concerns of accuracy and efficiency.

The notions of convergence, complexity, conditioning, compression, and orthogonality are among the most important of the big ideas. Any approximation method worth its salt must converge to the correct answer as more computational resources are devoted to it, and the complexity of a method is a measure of its use of these resources. The conditioning of a problem, or susceptibility to error magnification, is fundamental to knowing how it can be attacked. Many of the newest applications of numerical analysis strive to realize data in a shorter or compressed way. Finally, orthogonality is crucial for efficiency in many algorithms, and is irreplaceable where conditioning is an issue or compression is a goal.

In this book, the roles of the five concepts in modern numerical analysis are emphasized in short thematic elements called Spotlights. They comment on the topic at hand and make informal connections to other expressions of the same concept elsewhere in the book. We hope that highlighting the five concepts in such an explicit way functions as a Greek chorus, accentuating what is really crucial about the theory on the page.

Although it is common knowledge that the ideas of numerical analysis are vital to the practice of modern science and engineering, it never hurts to be obvious. The Reality Checks provide concrete examples of the way numerical methods lead to solutions of important scientific and technological problems. These extended applications were chosen to be timely and close to everyday experience. Although it is impossible (and probably undesirable) to present the full details of the problems, the Reality Checks attempt to go deeply enough to show how a technique or algorithm can leverage a small amount of mathematics into a great payoff in technological design and function. The Reality Checks proved to be extremely popular as a source of student projects in the first edition, and have been extended and amplified in the second edition.

NEW TO THIS EDITION. The second edition features a major expansion of methods for solving systems of equations. The Cholesky factorization has been added to Chapter 2 for the solution of symmetric positive-definite matrix equations. For large linear systems, discussion of the Krylov approach, including the GMRES method, has been added to Chapter 4, along with new material on the use of preconditioners for symmetric and nonsymmetric problems. Modified Gram–Schmidt orthogonalization and the Levenberg–Marquardt Method are new to this edition. The treatment of PDEs in Chapter 8 has been extended to nonlinear PDEs, including reaction-diffusion equations and pattern formation. Expository material has been revised for greater readability based on feedback from students, and new exercises and computer problems have been added throughout.

TECHNOLOGY. The software package MATLAB is used both for exposition of algorithms and as a suggested platform for student assignments and projects. The amount of MATLAB code provided in the text is carefully modulated, due to the fact that too much

tends to be counterproductive. More MATLAB code is found in the early chapters, allowing the reader to gain proficiency in a gradual manner. Where more elaborate code is provided (in the study of interpolation, and ordinary and partial differential equations, for example), the expectation is for the reader to use what is given as a jumping-off point to exploit and extend.

It is not essential that any particular computational platform be used with this textbook, but the growing presence of MATLAB in engineering and science departments shows that a common language can smooth over many potholes. With MATLAB, all of the interface problems—data input/output, plotting, and so on—are solved in one fell swoop. Data structure issues (for example those that arise when studying sparse matrix methods) are standardized by relying on appropriate commands. MATLAB has facilities for audio and image file input and output. Differential equations simulations are simple to realize due to the animation commands built into MATLAB. These goals can all be achieved in other ways. But it is helpful to have one package that will run on almost all operating systems and simplify the details so that students can focus on the real mathematical issues. Appendix B is a MATLAB tutorial that can be used as a first introduction to students, or as a reference for those already familiar.

The text has a companion website, `www.pearsonhighered.com/sauer`, that contains the MATLAB programs taken directly from the text. In addition, new material and updates will be posted for users to download.

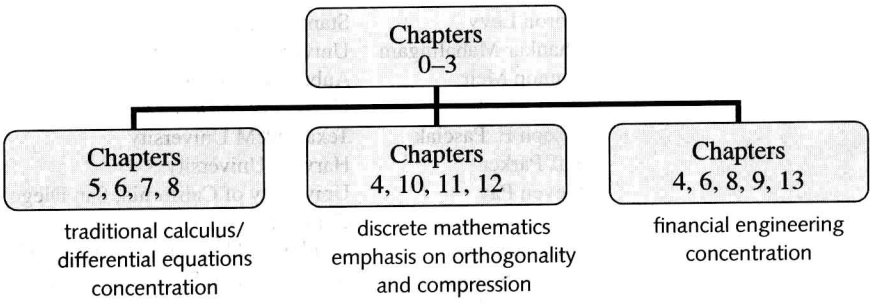
SUPPLEMENTS. To provide help for students, the **Student's Solutions Manual** (SSM: 0-321-78392) is available, with worked-out solutions to selected exercises. The **Instructor's Solutions Manual** (ISM: 0-321-783689) contains detailed solutions to the odd-numbered exercises, and answers to the even-numbered exercises. The manuals also show how to use MATLAB software as an aid to solving the types of problems that are presented in the Exercises and Computer Problems.

DESIGNING THE COURSE. *Numerical Analysis* is structured to move from foundational, elementary ideas at the outset to more sophisticated concepts later in the presentation. Chapter 0 provides fundamental building blocks for later use. Some instructors like to start at the beginning; others (including the author) prefer to start at Chapter 1 and fold in topics from Chapter 0 when required. Chapters 1 and 2 cover equation-solving in its various forms. Chapters 3 and 4 primarily treat the fitting of data, interpolation and least squares methods. In chapters 5–8, we return to the classical numerical analysis areas of continuous mathematics: numerical differentiation and integration, and the solution of ordinary and partial differential equations with initial and boundary conditions.

Chapter 9 develops random numbers in order to provide complementary methods to Chapters 5–8: the Monte-Carlo alternative to the standard numerical integration schemes and the counterpoint of stochastic differential equations are necessary when uncertainty is present in the model.

Compression is a core topic of numerical analysis, even though it often hides in plain sight in interpolation, least squares, and Fourier analysis. Modern compression techniques are featured in Chapters 10 and 11. In the former, the Fast Fourier Transform is treated as a device to carry out trigonometric interpolation, both in the exact and least squares sense. Links to audio compression are emphasized, and fully carried out in Chapter 11 on the Discrete Cosine Transform, the standard workhorse for modern audio and image compression. Chapter 12 on eigenvalues and singular values is also written to emphasize its connections to data compression, which are growing in importance in contemporary applications. Chapter 13 provides a short introduction to optimization techniques.

Numerical Analysis can also be used for a one-semester course with judicious choice of topics. Chapters 0–3 are fundamental for any course in the area. Separate one-semester tracks can be designed as follows:



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Contents

CHAPTER

0

Fundamentals

This introductory chapter provides basic building blocks necessary for the construction and understanding of the algorithms of the book. They include fundamental ideas of introductory calculus and function evaluation, the details of machine arithmetic as it is carried out on modern computers, and discussion of the loss of significant digits resulting from poorly-designed calculations.

After discussing efficient methods for evaluating polynomials, we study the binary number system, the representation of floating point numbers and the common protocols used for rounding. The effects of the small rounding errors on computations are magnified in ill-conditioned problems. The battle to limit these pernicious effects is a recurring theme throughout the rest of the chapters.

The goal of this book is to present and discuss methods of solving mathematical problems with computers. The most fundamental operations of arithmetic are addition and multiplication. These are also the operations needed to evaluate a polynomial $P(x)$ at a particular value x. It is no coincidence that polynomials are the basic building blocks for many computational techniques we will construct.

Because of this, it is important to know how to evaluate a polynomial. The reader probably already knows how and may consider spending time on such an easy problem slightly ridiculous! But the more basic an operation is, the more we stand to gain by doing it right. Therefore we will think about how to implement polynomial evaluation as efficiently as possible.

0.1 EVALUATING A POLYNOMIAL

What is the best way to evaluate

$$P(x) = 2x^4 + 3x^3 - 3x^2 + 5x - 1,$$

say, at $x = 1/2$? Assume that the coefficients of the polynomial and the number $1/2$ are stored in memory, and try to minimize the number of additions and multiplications required

to get $P(1/2)$. To simplify matters, we will not count time spent storing and fetching numbers to and from memory.

METHOD 1 The first and most straightforward approach is

$$P\left(\frac{1}{2}\right) = 2 * \frac{1}{2} * \frac{1}{2} * \frac{1}{2} * \frac{1}{2} + 3 * \frac{1}{2} * \frac{1}{2} * \frac{1}{2} - 3 * \frac{1}{2} * \frac{1}{2} + 5 * \frac{1}{2} - 1 = \frac{5}{4}. \quad (0.1)$$

The number of multiplications required is 10, together with 4 additions. Two of the additions are actually subtractions, but because subtraction can be viewed as adding a negative stored number, we will not worry about the difference.

There surely is a better way than (0.1). Effort is being duplicated—operations can be saved by eliminating the repeated multiplication by the input $1/2$. A better strategy is to first compute $(1/2)^4$, storing partial products as we go. That leads to the following method:

METHOD 2 Find the powers of the input number $x = 1/2$ first, and store them for future use:

$$\frac{1}{2} * \frac{1}{2} = \left(\frac{1}{2}\right)^2$$
$$\left(\frac{1}{2}\right)^2 * \frac{1}{2} = \left(\frac{1}{2}\right)^3$$
$$\left(\frac{1}{2}\right)^3 * \frac{1}{2} = \left(\frac{1}{2}\right)^4.$$

Now we can add up the terms:

$$P\left(\frac{1}{2}\right) = 2 * \left(\frac{1}{2}\right)^4 + 3 * \left(\frac{1}{2}\right)^3 - 3 * \left(\frac{1}{2}\right)^2 + 5 * \frac{1}{2} - 1 = \frac{5}{4}.$$

There are now 3 multiplications of $1/2$, along with 4 other multiplications. Counting up, we have reduced to 7 multiplications, with the same 4 additions. Is the reduction from 14 to 11 operations a significant improvement? If there is only one evaluation to be done, then probably not. Whether Method 1 or Method 2 is used, the answer will be available before you can lift your fingers from the computer keyboard. However, suppose the polynomial needs to be evaluated at different inputs x several times per second. Then the difference may be crucial to getting the information when it is needed.

Is this the best we can do for a degree 4 polynomial? It may be hard to imagine that we can eliminate three more operations, but we can. The best elementary method is the following one:

METHOD 3 (Nested Multiplication) Rewrite the polynomial so that it can be evaluated from the inside out:

$$\begin{aligned} P(x) &= -1 + x(5 - 3x + 3x^2 + 2x^3) \\ &= -1 + x(5 + x(-3 + 3x + 2x^2)) \\ &= -1 + x(5 + x(-3 + x(3 + 2x))) \\ &= -1 + x * (5 + x * (-3 + x * (3 + x * 2))). \end{aligned} \quad (0.2)$$

Here the polynomial is written backwards, and powers of x are factored out of the rest of the polynomial. Once you can see to write it this way—no computation is required to do the rewriting—the coefficients are unchanged. Now evaluate from the inside out:

$$\begin{aligned}
&\text{multiply } \frac{1}{2} * 2, \quad \text{add } +3 \to 4\\
&\text{multiply } \frac{1}{2} * 4, \quad \text{add } -3 \to -1\\
&\text{multiply } \frac{1}{2} * -1, \quad \text{add } +5 \to \frac{9}{2}\\
&\text{multiply } \frac{1}{2} * \frac{9}{2}, \quad \text{add } -1 \to \frac{5}{4}.
\end{aligned} \tag{0.3}$$

This method, called **nested multiplication** or **Horner's method**, evaluates the polynomial in 4 multiplications and 4 additions. A general degree d polynomial can be evaluated in d multiplications and d additions. Nested multiplication is closely related to synthetic division of polynomial arithmetic.

The example of polynomial evaluation is characteristic of the entire topic of computational methods for scientific computing. First, computers are very fast at doing very simple things. Second, it is important to do even simple tasks as efficiently as possible, since they may be executed many times. Third, the best way may not be the obvious way. Over the last half-century, the fields of numerical analysis and scientific computing, hand in hand with computer hardware technology, have developed efficient solution techniques to attack common problems.

While the standard form for a polynomial $c_1 + c_2x + c_3x^2 + c_4x^3 + c_5x^4$ can be written in nested form as

$$c_1 + x(c_2 + x(c_3 + x(c_4 + x(c_5)))), \tag{0.4}$$

some applications require a more general form. In particular, interpolation calculations in Chapter 3 will require the form

$$c_1 + (x - r_1)(c_2 + (x - r_2)(c_3 + (x - r_3)(c_4 + (x - r_4)(c_5)))), \tag{0.5}$$

where we call r_1, r_2, r_3, and r_4 the **base points**. Note that setting $r_1 = r_2 = r_3 = r_4 = 0$ in (0.5) recovers the original nested form (0.4).

The following MATLAB code implements the general form of nested multiplication (compare with (0.3)):

```
%Program 0.1 Nested multiplication
%Evaluates polynomial from nested form using Horner's Method
%Input: degree d of polynomial,
%       array of d+1 coefficients c (constant term first),
%       x-coordinate x at which to evaluate, and
%       array of d base points b, if needed
%Output: value y of polynomial at x
function y=nest(d,c,x,b)
if nargin<4, b=zeros(d,1); end
y=c(d+1);
for i=d:-1:1
  y = y.*(x-b(i))+c(i);
end
```

Running this MATLAB function is a matter of substituting the input data, which consist of the degree, coefficients, evaluation points, and base points. For example, polynomial (0.2) can be evaluated at $x = 1/2$ by the MATLAB command