普通高等学校“十三五”规划教材

数值分析

Numerical Analysis

（第2版）

苏岐芳　主编

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内 容 简 介

本书介绍了科学计算中常用数值分析的基础理论及计算机实现方法。主要内容包括：误差分析、插值、函数逼近、数值积分和数值微分、非线性方程的数值解法、线性方程组的直接解法、线性方程组的迭代解法、常微分方程的数值解法及相应的上机实验内容等。各章都配有大量的习题及上机实验题目，并附有部分习题的参考答案及数学专业软件 Mathematica 和 Matlab 的简介。

本书采用中、英两种语言编写，适合作为数学、计算机和其他理工类各专业本科“数值分析（计算方法）”双语课程的教材或参考书，也可供从事科学计算的相关技术人员参考。

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第 2 版前言

本书第 1 版出版以来，得到了许多专家、同仁及读者的关心、支持和帮助，并提出了许多宝贵意见和建议。借再版之机，首先向关心本书的广大读者、专家、同行和本书的各位责任编辑表示由衷的谢意！

在修订中，为了更适合当前双语教学的需求，我们保留了原教材的系统和编写风格（理论部分以英文为主，软件实现部分以中文为主），注意吸收当前国内外教材改革中一些成功的经验，努力体现创新教学理念，以利于激发学生自主学习，提高实践应用能力，培养综合素质和创新能力。

本次再版修订的内容主要包括以下几方面：

1. 订正了语言文字表达方面的不足之处，力求用词规范，表达确切。

2. 剔除了个别内容重复和烦琐之处，使理论部分更好地体现“够用为度”的编写原则。

3. 恰当地处理有关定理的证明和有关例题的求解方法，使其更加通俗易懂。

4. 增补了多重积分、有理逼近、Padé 逼近等内容，进一步体现教材的先进性。

5. 结合增补内容，对习题配置作了进一步充实、完善。

6. 在实验部分，大量增加了算法的 Matlab 实现程序及相应的算例，以便于指导学生实践应用。

本书由浙江台州学院苏岐芳副教授主编，浙江台州学院郑学良教授、李希文副教授和应玮婷老师参与修订。具体写作分工为：第 1 章、第 2 章及附录由李希文修订；第 3 章由郑学良修订；第 4 章~第 8 章由苏岐芳修订；全书的计算机实验由应玮婷修订。

在本书修订过程中，浙江师范大学徐秀斌教授为本书提出了许多宝贵意见，在此表示衷心感谢！

编　者

2016 年 10 月

第 1 版前言

数值分析（计算方法），是研究数学问题数值解的构造性方法的一门科学。它既具有纯数学理论的抽象性和严谨性，更具有实用性和实验性的技术特征，是一门理论性和实践性都很强的学科。

随着计算机和计算方法的飞速发展，几乎所有学科都走向定量化和精确化，从而产生了一系列计算性的学科分支，如计算物理、计算化学、计算生物学、计算地质学、计算气象学和计算材料学等，计算数学中的数值计算方法则是解决“计算”问题的桥梁和工具。在科学研究和工程技术中都要用到各种计算方法。例如，在航天航空、地质勘探、汽车制造、桥梁设计、天气预报和汉字字样设计中都有计算方法的踪影。

在二十世纪七八十年代，大多数高校仅在数学系的计算数学专业和计算机系开设计算方法这门课程。现在，计算方法课程几乎已成为所有理工科学生的必修课程。在计算机上采用数值计算方法解决科学与工程计算中的实际问题已成为当今科学实验与理论研究的重要手段，利用计算机求解各类数学问题数值解的能力，已成为广大科技工作者、大学生和各类管理人员必备的能力。

本书是在作者多年来开设“数值分析”双语教学讲义的基础上，吸收国内外同类教材的精华，采用中英文双语编写而成。主要介绍了计算机中常用的、有效的各类数值问题的计算方法及相关数学理论。全书共分八章，包括误差分析、插值、函数逼近、数值积分和数值微分、非线性方程的数值解法、线性方程组的直接解法、线性方程组的迭代解法、常微分方程的数值解法等内容。每章由开篇、理论、应用和习题四个部分构成。

每章的开篇部分，给出中文内容提要和主要英语词汇解释，通过具体案例引入本章话题并提出本章的学习目标；理论部分以英文为主，重要的名词术语同时标注中文，从而**使读者在方便、有效地掌握知识的同时，渐进提高专业英语的阅读和应用能力。这是本书的第一个特点**。

每章的应用部分，采用算法分析、计算机示范程序、计算实例的结构安排，逐步引导读者将理论和方法转化为实际操作，并应用专业计算机软件实现更为复

杂的数值计算，从而**培养读者利用计算机解决数学问题的能力**。这是本书的**第二个特点**。

每章还配备了大量的理论分析和计算机实验题目，书末附有部分习题参考答案及专业软件介绍，可以满足不同学习层次读者的学习需求；同时，还可以启发读者使用不同的计算机语言编写计算程序。**既体现了学习的自主性，又有利于培养读者的动手能力与创新能力**。这是本书的**第三个特点**。

本书由浙江台州学院苏岐芳主编，中欧国际工商学院苏岐英主审。各章编写情况如下：苏岐芳编写第1～5章，郑学良编写第6、7章，浙江海洋学院郝彦编写第8章，浙江台州学院李希文编写全书的计算机实验内容及附录。另外，浙江台州学院陈淑萍和浙江海洋学院朱玉辉对本书的编写也做了大量工作，在此一并致谢。

在本书的编写过程中，参阅了大量的文献，在此对这些作者表示衷心感谢！限于水平，书中错误和不足之处在所难免，恳请专家、教学同仁和广大读者批评指正，提出宝贵意见。

编　者

2007年2月

Contents

1 Error Analysis

提 要

本章主要介绍误差的来源、绝对误差和相对误差、误差的传播规律，以及数值计算中控制误差的一些原则等.

词 汇

accuracy	精度	integral	积分
absolute error	绝对误差	multiplication	乘法
algorithm	算法	polynomial	多项式
convergence	收敛性	round-off error	舍入误差
decimal	十进制 (小数)	relative error	相对误差
discard	抛弃,舍弃	stability	稳定性
division	除法	series	级数
disturbance	扰动	significant digits	有效数字
elimination	消元	subtraction	减法
function	函数	truncation error	截断误差

1.1 Introduction

Although the computer is an ideal tool for performing complex numerical computations, casual or careless use of the output from a computer program can lead to highly undesirable **consequences** (推论). Indeed, one of the most common mistakes made by new users is to accept, almost as a matter of faith, the validity of numerical output produced by an operational computer program. A relatively begin **manifestation** (显示) of this phenomenon arises when one attributes more **precision** (精确) to a numerical output than the accuracy of the input data or the underlying mathematical model justifies.

In other instances, a value produced by an operational computer program can be totally meaningless in the sense that is not accurate to even one digit. This can result from an **accumulation** (累积) of round-off error due to the way a calculation is structured. As a simple illustration, consider the following **quadratic equation** (二次方程).

$$ax^2 + bx + c = 0 \tag{1.1.1}$$

Note that this equation is labeled (1.1.1) where the first digit identifies the chapter, the second digit identifies the section within in the chapter, and the last digit identifies the equation within in the section.

Suppose we want to find the two roots of (1.1.1). Using the well-known quadratic formula, the roots are

$$x_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \tag{1.1.2}$$

To make the problem more specific, suppose the parameters are $a = 1, b = -(10^4 + 10^{-4})$, and $c = 1$. Carrying out the calculation in (1.1.2) yields the roots $x_1 = 10^4$ and $x_2 = 10^{-4}$. Interestingly enough, if we perform this simple calculation on a computer that has a precision of seven decimal digits (not uncommon), then the results are $x_1 \approx 10^4$ and $x_2 = 0$. That is, the first root is easily obtained, but the error in the second root is 100 percent! This is a consequence of accumulated round-off error.

When you finish this chapter, you will know how the principal sources of error in numerical computations arise, including round-off error and formula truncation error. You will know how to control the **propagation** (传播) of errors. You will understand the significant digits of approximate number. You will achieve these overall goals by mastering the following chapter objectives.

Objectives

- Know how to define, calculate, and use the absolute and relative errors.
- Understand how round-off error and truncation error occur.
- Be able to analyze error propagation in basic arithmetic operations.
- Be able to specify bounds on the size of formula truncation error.
- Know how to choose proper algorithm for some mathematical model.

1.2 Sources of Errors（误差的来源）

Assessing (估计) the accuracy of the results of calculations is a paramount goal in numerical analysis. One distinguishes several kinds of errors which may limit this accuracy:

1. model errors（模型误差）

When we use computer to calculate a mathematical problem, we first set up a mathematical model which is **abstraction** (抽象化) and **simplification** (简单化) of the described practical problem, it is approximate. We call the error between mathematical model and practical problem **model error.**

Example 1.2.1

$$s(t)=\frac{1}{2}gt^2,\quad g\approx 9.812$$

2. Errors in the input data（输入数据误差）

Input data errors are beyond the control of the calculation. They may be due, for instance, to the inherent imperfections of physical measurements.

3. Round-off errors（舍入误差）

Round-off errors arise if one calculates with numbers whose representation is restricted to a finite number of digits, as is usually the case.

Rounding is an important concept in scientific computing. Consider a positive decimal number x of the form 0.□□□···□□□ with m digits to the right of the **decimal point** (小数点). One rounds x to n decimal places ($n<m$) in a manner that depends on the value of the (n+1)st digit. If this digit is a 0, 1, 2, 3, or 4, then the nth digit is not changed and all following digits are **discarded** (抛弃,舍弃). If it is a 5, 6, 7, 8 or 9, then the nth digit is increased by one unit and the remaining digits are discarded.

Here are some examples of seven-digit numbers being correctly rounded to four-digits

$$0.162\,5\leftarrow 0.162\,548\,9$$

$$1.000\quad\leftarrow 0.999\,960\,1$$

$$0.623\,3\leftarrow 0.623\,270\,9$$

If x is rounded so that $\bar{x}$ is the n-digit approximation to it, then

$$\left|x-\bar{x}\right|\leqslant\frac{1}{2}\times 10^{-n}$$

Another example, $\pi=3.141\,592\,6\cdots$, if we take $\pi\approx 3.14$, then the round-off error is $3.14-3.141\,592\,6\cdots=-0.001\,592\,6\cdots$.

4. Truncation errors（截断误差）

As for the fourth kind of the error, many methods will not yield the exact solution of the given problem, even if the calculations are carried out without rounding, but rather the solution of another simpler problem $\bar{P}$ which approximates P. For instance, the problem P of summing an infinite series, e.g.(例如),

$$\sin x=x-\frac{x^3}{3!}+\frac{x^5}{5!}-\frac{x^7}{7!}+\cdots$$

may be replaced by the simpler problem $\bar{P}$ of summing only up to a finite number of terms of the series.

$$\sin x\approx x-\frac{x^3}{3!}+\frac{x^5}{5!}-\frac{x^7}{7!}$$

The resulting approximation error is commonly called a **truncation error**.

Generally, $f(x)$ can be approximately replaced by **Taylor polynomial** (泰勒多项式)

$$P_n(x) = f(0) + \frac{f'(0)}{1!}x + \frac{f''(0)}{2!}x^2 + \cdots + \frac{f^{(n)}(0)}{n!}x^n$$

the truncation error is

$$R_n(x) = f(x) - P_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}x^{n+1}$$

where ξ is between 0 and x .In this book,"ξ is between a and b" means that either $a<\xi<b$ or $b<\xi<a$.

1.3 Errors and Significant Digits（误差和有效数字）

Definition 1.3.1 If a real number x^* approximates to another number x, then the **absolute error (or error)** (绝对误差) is defined by

$$e = x^* - x$$

where e may be positive or negative number. If the absolute error is positive, the **approximate value** (近似值) is greater than the **exact value** (准确值), it is called **strong approximate value** . If the absolute error is negative, the approximate value is smaller than the exact value, it is called **weak approximate value** .

If there exists a positive number ε, such that

$$|e| = |x^* - x| \leqslant \varepsilon$$

Then ε is called the **limit of the (absolute) error** (绝对误差限). That is

$$x^* - \varepsilon \leqslant x \leqslant x^* + \varepsilon \quad \text{or} \quad x = x^* \pm \varepsilon$$

Example 1.3.1 The representation $x = 0.310\,6 \pm 0.001\,4$ implies

$$0.310\,6 - 0.001\,4 \leqslant x \leqslant 0.310\,6 + 0.001\,4$$

That is

$$0.309\,2 \leqslant x \leqslant 0.312\,0$$

Example 1.3.2 We measure the length of an object with **mm-graduation ruler** (毫米单位刻度尺), then

$$|e| = |l^* - l| \leqslant \frac{1}{2}\ \text{mm}$$

If the reading is $l^* = 513\ \text{mm}$, then $512.5\ \text{mm} \leqslant l \leqslant 513.5\ \text{mm}$.

Example 1.3.3 Discuss the calculation of e^{-x} for $0 < x < 1$ from the **series** (级数)

$$\mathrm{e}^{-x} = 1 - \frac{x}{1!} + \frac{x^2}{2!} - \frac{1}{3!}x^3 \cdots + \frac{(-x)^n}{n!} + \cdots$$

Solution Let

$$E(x) = 1 - \frac{x}{1!} + \frac{x^2}{2!} - \frac{1}{3!}x^3$$

Then

$$\left|e^{-x}-E(x)\right| \leqslant \frac{1}{24}$$

The limit of the error is $\frac{1}{24}$.

Definition 1.3.2 If a real number x^* approximates to another number x, then the **relative error** (相对误差) of x^* is

$$e_r = \frac{e}{x} = \frac{x^* - x}{x}$$

Frequently

$$e_r = \frac{e}{x^*} = \frac{x^* - x}{x^*}$$

If there exists a positive number ε_r, such that

$$|e_r| \leqslant \varepsilon_r$$

Then ε_r is called the **limit of relative error** (相对误差限).

Example 1.3.4 If $x = 10 \pm 1, \quad y = 1000 \pm 5$

Then

$$x^* = 10, \ \varepsilon(x) = 1, \ y^* = 1\,000, \ \varepsilon(y) = 5$$

$$\varepsilon_r(x) = \frac{\varepsilon(x)}{|x^*|} = 10\%, \quad \varepsilon_r(y) = \frac{\varepsilon(y)}{|y^*|} = 0.5\%$$

Example 1.3.5 $x = \pi = 3.141\,592\,65\cdots$.

If $x_3^* = 3.14$, then $\varepsilon_3^* \leqslant 0.002$; if $x_5^* = 3.141\,6$, then $\varepsilon_5^* \leqslant 0.000\,05$. We can see that the errors do not exceed the half unit of their end places . i.e.,

$$|\pi - 3.14| \leqslant \frac{1}{2} \times 10^{-2}, \qquad |\pi - 3.141\,6| \leqslant \frac{1}{2} \times 10^{-4}$$

Definition 1.3.3 If the limit of the error of approximate value x^* is a half unit of some place, and there are n digits from this place to the first nonzero digit of the front of x^*, then we say x^* has n **significant digits** (or **figures**).

x^* can be represented:

$$x^* = \pm 10^m \times (a_1 + a_2 \times 10^{-1} + \cdots + a_n \times 10^{-(n-1)}) \tag{1.3.1}$$

where $a_i \in \{0,1,2,\cdots,9\} (i = 1,\cdots,n)$, and $a_1 \neq 0$, m is an **integer** (整数), furthermore

$$\left|x - x^*\right| \leqslant \frac{1}{2} \times 10^{m-n+1} \tag{1.3.2}$$

e.g.,

$$31.415 = 10^1 \times (3 + 1 \times 10^{-1} + 4 \times 10^{-2} + 1 \times 10^{-3} + 5 \times 10^{-4})$$

where $m = 1, n = 5, \left|x - x^*\right| \leqslant \frac{1}{2} \times 10^{-3}$.

Example 1.3.6 Let $x^* = 3.14$ be the approximate value of π, then it has three significant digits. Let $x^* = 3.141\,6$ be the approximate value of π, then it has five significant digits.

Example 1.3.7 Write the approximate numbers with five significant digits of the following numbers by rounding-off

$$187.932\,5,\quad 0.037\,856,\quad 8.000\,0,\quad 2.718\,281\,8$$

Solution The results are respectively

$$187.93,\quad 0.037\,856,\quad 8.000\,0,\quad 2.718\,3$$

Example 1.3.8 Let $g \approx 9.80\ \mathrm{m/s^2}$, $g \approx 0.009\,80\ \mathrm{km/s^2}$. Then they have three significant digits, and

$$|g-9.80| \leqslant \frac{1}{2}\times 10^{-2},\qquad \text{where } m=0, n=3.$$

$$|g-0.009\,80| \leqslant \frac{1}{2}\times 10^{-5},\quad \text{where } m=-3, n=3.$$

Their limits of the absolute errors are different,

$$\varepsilon_1 = \frac{1}{2}\times 10^{-2}\,\mathrm{m/s^2},\qquad \varepsilon_2 = \frac{1}{2}\times 10^{-5}\,\mathrm{km/s^2}$$

and their relative errors are equal,

$$\varepsilon_r = 0.005/9.8 = 0.000\,005/0.009\,80$$

Remarks 1.3.1

(1) The number of significant digits is not relative to the place of the decimal point, e.g., both 3.14 and 314 have three significant digits.

(2) From $|x-x^*| \leqslant \frac{1}{2}\times 10^{m-n+1}$, we obtain that the more significant digits an approximate number has, the smaller limit of the absolute error it has.

(3) Zero at the end of an approximate number can not be **rounded down** (舍去).

Theorem 1.3.1 Let approximate number x^* be represented by

$$x^* = \pm 10^m \times (a_1 + a_2\times 10^{-1} + \cdots + a_n \times 10^{-(n-1)})$$

where $a_i (i=1,\cdots,n)$ is one of the digits from 0 to 9, $a_1 \neq 0$, m is an integer . If x^* has n significant digits , then its limit of the relative error satisfies

$$\varepsilon_r \leqslant \frac{1}{2a_1}\times 10^{-(n-1)}$$

Contrarily, if the limit of the relative error of x^* satisfies

$$\varepsilon_r \leqslant \frac{1}{2(a_1+1)}\times 10^{-(n-1)}$$

then x^* has n significant digits at least.

Proof Using (1.3.1) $x^* = \pm 10^m \times (a_1 + a_2\times 10^{-1} + \cdots + a_n \times 10^{-(n-1)})$

we obtain

$$a_1 \times 10^m \leqslant |x^*| < (a_1+1)\times 10^m$$

If x^* has n significant digits, then