

COMPUTATIONAL MATHEMATICS

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Preface

The rapid development of computer engineering in recent times has led to an expansion of application of mathematics. Quantitative methods have been introduced into practically every sphere of human activity. The use of computers in the economy requires skilled specialists who have a command of the methods of computational mathematics.

Computational mathematics is one of the principal disciplines necessary for the preparation of specialists for various branches of economy. By studying it students acquire theoretical knowledge and practical skill to solve various applied problems with the aid of mathematical models and numerical methods that are realized on a computer.

This study aid assumes that the reader is aware of the elementary concepts of higher mathematics, i.e. continuity, the derivative and the integral. It covers three large divisions of mathematics: "Algebraic Methods" (Ch. 2-6), "Numerical Methods of Analysis" (Ch. 1, 7, 8) and "Numerical Methods of Solving Differential Equations" (Ch. 9, 10).

The theoretical material presented is illustrated by numerous examples. Each chapter is concluded by exercises for independent work.

The following designations are used in the book: the signs \square and \blacksquare are used for the beginning and end of the proof of an assertion and the signs \triangle and \blacktriangle for the beginning and end of the solution of a problem.

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Authors

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Introduction

Before beginning the exposition of the material, we shall briefly characterize computational mathematics, for which purpose we shall answer the following three questions:

(1) What is computational mathematics?

(2) What are the distinctive features of computational mathematics which allow it to be a special division of mathematics?

(3) What is the significance of computational mathematics for the economy?

1. The term "computational mathematics" means now a division of mathematics which studies problems connected with the use of computers.

We can distinguish three trends in computational mathematics. The first trend is connected with the use of computers in various fields of research and applications and includes, in particular, numerical solution of various mathematical problems. The second trend is connected with the elaboration of new numerical methods and algorithms and perfecting the old ones. The third trend is connected with the problems of the interaction of man and computer.

This book is devoted to the first trend, namely, the use of numerical methods when solving applied problems.

The foundation on which computational mathematics is constructed is composed of various computing facilities, computers first of all, whose rapid development is the most characteristic feature of the technological progress today. Thus, during the last thirty years, the speed of computation increased from one operation per second (with the use of a slide rule) to 3 000 000 operations per second, i.e. $3 \cdot 10^6$ times. It is appropriate to

recall that from the time when a steam engine was invented the speed of travel increased from 13 km per hour (the speed of a horse) to 40 000 km per hour (the speed of a cosmic vehicle), i.e. only $3 \cdot 10^3$ times.

2. We can use the following examples to illustrate the characteristic features of computational mathematics which distinguish it from pure mathematics.

From the point of view of a "pure" mathematician, to solve a problem is to prove the existence of its solution and show a process which leads to a solution. For a programmer, the time of obtaining a solution, i.e. the rate of convergence of the process, is often a more important factor. Thus, it is known that a solution of n simultaneous algebraic equations can be theoretically obtained for any specified n as a result of a finite number of operations, say, with the aid of the method of Cramer or Gauss. Therefore, from the viewpoint of a "pure" mathematician, a problem of this kind is considered to be solved. However, when these methods are used in practical applications, two difficulties, which can not always be overcome, are often encountered. The first difficulty is that for a sufficiently large n the number of operations, although finite, is so large that it is impossible to carry out all of them even with the use of the most powerful computers. Thus, to solve a system of n equations by Cramer's method, we must perform $n \cdot n!$ operations, and this constitutes $4.6 \cdot 10^{19}$ operations for $n = 20$. Then, with the rate of $3 \cdot 10^6$ operations per second a computer must operate continuously for half a million years. Gauss' method proves to be more efficient. With the use of this method, the number of operations needed to solve the same problem is of the order of n^3 .

However, such a large number of operations generates a second principal difficulty: the errors resulting from all operations accumulate and exert such a great influence on the final result that it often becomes far distant from the true solution.

Nowadays exact methods are usually used for solving systems of equations when their order is not higher than 10^3 . Therefore, from the point of view of a programmer, the problem of solving a system whose order is higher than 10^3 is not at all trivial. To solve such a system, ite-

rative methods are used which are approximate but possess a significant advantage of not accumulating computational errors from iteration to iteration. Thus we deal with a seemingly paradoxical situation, but one that is typical of numerical methods, namely, that approximate algorithms are preferred to exact ones.

3. The essential expansion of the fields of application of computational mathematics, including its inculcation into economy, can be explained by the fact that natural phenomena and the phenomena of social life, different in their sense, are often similar in formal structure and can, consequently, be described by the same mathematical models. We can therefore use the same numerical methods to solve the problems described by these models.

Computers are principal factors making for the acceleration of the scientific and technical progress, for the realization of the complex and purposeful programs of solution of the most important scientific and technological problems and for the further increase in the productivity of labour. The development of computers and computational mathematics will make it possible, for instance, to pass from the automatization of the control of technological systems and processes to the automatization of the control of production processes.

Chapter 1

Elementary Theory of Errors

1.1. Exact and Approximate Numbers. Sources and Classification of Errors

In the process of solving a problem, we have to deal with various numbers which may be exact or approximate. Exact numbers give a true value of a number and approximate numbers give a value close to the true one, the degree of closeness being dependent on the error of calculation.

For example, in the assertions “a cube has six faces”, “we have five fingers to a hand”, “there are 32 students in a class”, “there are 582 pages in a book” the numbers 6, 5, 32 and 582 are exact ones. In the assertions “the house is 14.25 m wide”, “the radius of the Earth is 6000 km”, “the mass of a match box is ten g” the numbers 14.25, 6000 and 10 are approximate.

This is due, first of all, to the imperfection of measuring instruments we use. There are no absolutely exact measuring instruments, each of them has its own accuracy, i.e. admits of a certain error of measurements. In addition, in the second example the approximation of a number is in the very concept of the radius of the Earth. The matter is that, strictly speaking, the Earth is not a sphere and we can speak of its radius only in approximate terms. In the next example, the approximation of the number is also defined by the fact that different boxes may have different masses and the number 10 defines the mass of a certain box.

In other cases, the same number may be exact as well as approximate. Thus, for instance, the number 3 is exact if we speak of the number of sides of a triangle and approximate if we use it instead of the number π when calculating the area of a circle using the formula $S = \pi R^2$.

In practical calculations, we understand the *approximate number* a to be a number which differs but slightly

from the exact number A and can be substituted for it in calculations.

The solution of the majority of practical problems with a certain degree of conventionality can be represented as two successive stages: (1) the mathematical description of the problem on hand, (2) the solution of the formulated mathematical problem.

At the first stage, we may encounter two characteristic sources of errors. First, the fact that the processes happening in reality can not always be described by means of mathematics and the simplifications we introduce make it possible to obtain only more or less idealized models. Second, the initial parameters are, as a rule, inexact since they are obtained from an experiment which gives only an approximate result.

Accordingly, the total error of a mathematical model and initial data is considered to be the *error of the initial information*. Having in mind that this error is independent of the second stage of solving the problem, we often call it a *nonremovable error*.

It is, as a rule, unrealizable in practice to obtain an exact solution of a mathematical problem (the second stage) irrespective of whether it is constructed analytically or on a computer. Thus, for instance, we can obtain an exact solution for only a very restricted class of differential equations. Therefore, in practical calculations, we usually use the methods of approximation of solutions, numerical first of all.

Such a compulsory replacement of an exact solution by an approximate one generates an *error of the method* or, as it is often called, an *error of approximation*.

Finally, in the process of problem solving, we round off the initial data as well as the intermediate and final results. These errors and the errors arising in the arithmetic operations involving approximate numbers affect, more or less, the result of calculations and form a so-called *rounding error*.

In this connection, when we formulate a problem, we either indicate the accuracy of the solution required, i.e. specify the maximum error permissible in all calculations, or only calculate the total error of the result. Therefore, when dealing with approximate numbers, it is

necessary to know how to solve the following problems:

- (1) to characterize the exactness of approximate numbers by mathematical means,
- (2) to estimate the degree of accuracy of the result when we know the degree of accuracy of the initial data,
- (3) to choose initial data with the degree of accuracy which will ensure the specified accuracy of the result,
- (4) to construct an optimal computing process in order to obviate the calculations which do not affect the valid digits of the result.

1.2. Decimal Notation and Rounding off Numbers

Every decimal positive number a can be represented as a finite or infinite decimal fraction

$$a = \alpha_1 \cdot 10^m + \alpha_2 \cdot 10^{m-1} + \dots + \alpha_n \cdot 10^{m-n+1} + \dots, \quad (1)$$

where α_i are the digits constituting the number ($i = 1, 2, \dots, n, \dots$) with $\alpha_1 \neq 0$, and m is the top digit in the number a .

Example 1. Represent the number 1905.0778 in form (1):

$$\begin{aligned} 1905.0778 = & 1 \cdot 10^3 + 9 \cdot 10^2 + 0 \cdot 10^1 + 5 \cdot 10^0 + 0 \cdot 10^{-1} \\ & + 7 \cdot 10^{-2} + 7 \cdot 10^{-3} + 8 \cdot 10^{-4}. \end{aligned}$$

Every unit in the corresponding i th decimal position, reckoning from left to right, has its value 10^{m-i+1} known as the *value of the decimal position*. Thus the value of the first (from the left) decimal position is 10^m , that of the second is 10^{m-1} and so on.

In the example considered, the value of the decimal position containing the digit 9 is $10^{3-2+1} = 100$, of that containing the digit 5 is $10^{3-4+1} = 1$, of that containing the digit 8 is $10^{3-8+1} = 0.0001$.

In practical calculations we often have to round off a number, i.e. to replace it by another number consisting of a smaller number of digits. In that case we retain one or several digits, reckoning from left to right, and discard all the others.

The following *rules of rounding off* are most often used.

1°. If the discarded digits constitute a number which is larger than half the unit in the last decimal place that remains, then the last digit that is left is strengthened (increased by unity).