SHAN S. KUO

COMPUTER
APPLICATIONS
OF
NUMERICAL
METHODS

Computer Applications of Numerical Methods

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Computer Applications of Numerical Methods

To my parents

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Preface

During the past fourteen years the author has been giving a course in numerical methods and computers at Yale and Tufts Universities and the University of New Hampshire. This course is designed to acquaint students with the numerical methods used in solving problems by means of a high-speed digital computer. The interests of his audience have included such diverse subjects as biology, chemical engineering, chemistry, civil engineering, economics, electrical engineering, computer science, mechanical engineering, physics, psychology, and pure mathematics.

When I began teaching this course, I found that many excellent texts in numerical methods were available, but most of them were either not computer-based or were too specialized for use in a course of this nature. Furthermore, most books in programming languages touched little on numerical methods. Accordingly, it became necessary to prepare some mimeographed notes from which this book developed.

In preparing these lecture notes, I had two objectives in mind: first, to provide the student with the necessary fundamental knowledge of the computer-oriented numerical methods for basic problems in algebra and analysis which form the building blocks for more complicated problems; second, to acquaint him with a high-speed digital computer. The student was required to program and solve meaningful problems on a computer. Experience in the classroom has indicated that this approach develops an excellent comprehension of the successful application of computer-oriented numerical methods.

This text is divided into three parts. Part I deals with man-machine communication in some detail. Part II describes the various numerical methods that have been proved suitable for electronic computers. Part III is concerned with modern topics in digital computation, including linear programming and the Monte Carlo method.

The book is a revision of *Numerical Methods and Computers*, published in 1965. In preparing it the popular IBM System/360 and its Basic FORTRAN IV language

are used for illustrative purposes. Programs written in this subset of the language can be implemented on the IBM System/360, System/370, and many other computers. This subset of FORTRAN language is compatible with and encompasses American Standard Association (ASA) Basic FORTRAN.

This book incorporates not only some new material, but also additional problems as well as a very substantial number of new references. Chapters 2, 4, and 5, as well as every FORTRAN program in the book, have been entirely rewritten. I have added detailed discussions of Romberg's method in Chapter 12, propagation of error from initial data in Chapter 13, and dumps in Appendix B. Two new sections have also been added to Chapter 14 in connection with the generation of pseudo random numbers by the multiplicative congruence method.

The book is suited for courses on the methods of modern computation which are included in the curricula of most universities. The prerequisite in methematics is a good knowledge of calculus and, preferably, elementary differential equations. It is hoped that this book forms a bridge between programming techniques and methods of numerical analysis. The deliberate emphasis on the flow chart and the presentation of a tested FORTRAN program for each numerical method should provide the student with real insight into the techniques of computer problem solving, and scientists and engineers with a guide to the solution of advanced problems.

It is with pleasure that I gratefully acknowledge the help and encouragement of my friends, colleagues, and students. In particular, my thanks go to D. T. Chin, C. S. Chu, W. D'Avanzo, R. Desmaison, D. S. Fine, Y. W. Hsu, L. P. Kuan, J. M. Lee, G. H. Room, R. O. Sather, J. Stephenson, E. Vaines, L. A. Walsh, and C. Wolfe for their comments, criticisms, and help in eliminating errors. I also wish to express my appreciation to Drs. A. Wang and S. Chao for helpful comments on Chapter 2. Numerous ideas were drawn from the internal publications of Computation Centers at Dartmouth College, Massachusetts Institute of Technology, University of Michigan, University of New Hampshire, Tufts University, and Yale University.

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Durham, New Hampshire December 1971

S.S.K.

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COMMUNICATION WITH DIGITAL COMPUTERS

The subject matter of Part I is concerned with an introduction of computer components and the general problem of man-machine communication. It is divided into five chapters. Chapter 1 is introductory in aim and content while Chapter 2 deals with the basic units of digital computers. Chapter 3 represents logical flow charting, a graphical representation of a sequence of commands. Chapter 4 is concerned with the floating-point method of arithmetic. Chapter 5 presents the FORTRAN coding system together with many detailed examples.

Introduction

1.1 CHARACTERISTICS OF DIGITAL COMPUTERS

High-speed electronic computers are triggering a revolution in the solving of engineering and science problems. This revolution will free men from many mentally stultifying computational tasks, and more important, it will make possible the solution of engineering and science problems of greater complexity.

There are two classes of computers: analog and digital. An analog computer, like a slide rule, solves problems by converting numbers into physical quantities such as distance or electrical resistance. On the other hand, a high-speed digital computer is like a desk calculator in that it uses numbers to express all the variables and quantities of a problem. However, it differs from a desk calculator in one important respect: It can automatically perform a long and complete sequence of operations without intervention from the human operator.

This book deals exclusively with digital computations; references to analog computations are listed at the end of the chapter.

We shall now discuss some marked characteristics of digital computers, the first of which is their high speed. In a matter of seconds or minutes, vast quantities of computations can be automatically performed. Computations avoided because of their impracticality prior to the use of digital computers can now be handled as a matter of simple routine. Consider the case of comparative engineering design. The designer, without computers, would either make a "guestimate" from his experience or at best estimate only one or two alternatives. When a digital computer is used, a complete comparative study can be obtained to show the effect of numerous parameters in a short time.

The digital computer is not merely a glorified slide rule; it has the ability to store, or remember, various information for future use. Such information includes the

4 Introduction 1.2

original data, commands of operation, and intermediate results. In addition, digital computers are able to change or modify the commands of operations internally, and frequently the intermediate results obtained are used internally to dictate the path of subsequent computations.

For example, at a point of computation, the answer is tested for zero. Depending on whether or not the answer is zero, the machine will automatically take one of two entirely different courses for subsequent computations. Thus the digital computer is also noted for its ability to make a logical decision.

1.2 A BRIEF HISTORY AND SURVEY OF THE APPLICATION OF DIGITAL COMPUTERS

The first all-electronic digital computer was completed in 1946 at the University of Pennsylvania and was named the Electrical Numerical Integrator and Automatic Computer (ENIAC). Vacuum tubes were used for most of its functions. This was a great improvement over the Mark I digital computer built at Harvard University in 1944, which made use of electromechanical relays.

In the period following the completion of the ENIAC, two significant developments made possible the present-day family of computers. One was the development of a memory device for holding a few hundred to several thousand numbers. The other was the realization that commands could also be stored in this memory device in a manner similar to that in which the numbers are stored. This knowledge made it possible to instruct the computer to follow these commands from each memory space as required. In the meantime, the representation of numbers in the binary system was put in use, and since that time the number of basic commands has been steadily increased. The vacuum tube computers constituted the first generation, from 1947 to about 1959.

Since 1951 there have been continuous advances in the design and components of digital computers. Among these were the introduction of solid-state or transistorized design, increased number of available memory spaces, faster speed of operation, and a further diversification of commands. The second generation of computers, characterized by the solid-state design, began to appear in the market in 1959.

Many super computers have been built since 1951, including LARC, Stretch, CDC 6600, 7600, and ILLIAC IV. They have been designed to reach to the limit of existing practice in terms of speed, size, and logic design.

Most computers built since 1965 belong to a third generation. These computers are characterized by the microelectronics technology (electronic chips) in hardware and multiprocessor multiprogramming systems in software.

Digital computers are presently being used to store and retrieve information quickly and economically, simulate complex business operations, create a "model" river system, help determine who wrote the Federalist papers whose authorship is disputed, chart the complex interrelations among the hundreds of electric signals reproduced by the living brain, formulate and prove mathematical theorems, take the first step toward translation of languages, forecast the weather, and analyze the decay tracks left by strange particles in bubble chambers.

Computers are also used to calculate spacecraft orbits, process payrolls, update transactions, control chemical blending processes, design structures and machine components, and assist in medical diagnoses. They are simulating aircraft flight characteristics, automating airline reservation procedures, and controlling inventories. Two-way communication between the brain of a chimpanzee and a computer has also been established.

A procedure called *time-sharing* which brings the user closer to the computer is rapidly gaining recognition. In this procedure, a number of consoles scattered in different locations are connected to one central computer so that a number of users can take over control, successively, as they need its services. While the large time-sharing systems are subject to continuing research, the use of conventional computers by means of on-line remote consoles may well be an important consideration in future development.

Another interesting development is in the area of engineering graphics. By using a light pen on a cathode-ray oscilloscope, one can draw two projections of a given object and ask the computer to straighten out lines or rectify angles. A perspective view can then be produced by the computer and, if desired, recorded on microfilm. Similarly, the equation of a surface may be read in and a contour plot can readily be made by the computer.

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