A SURVEY OF NUMERICAL ANALYSIS

Edited by

JOHN TODD

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Preface

Origins

In 1957 a grant was made to the National Bureau of Standards, by the National Science Foundation, for the support of a Training Program in Numerical Analysis for Senior University Staff, under my direction. An objective of this program was to attract mature mathematicians into an area of vital importance which had been largely neglected. The first chapter of this book tries to show that numerical analysis is an attractive subject in which mathematics of practically all sorts can be used significantly, and from which many branches of mathematics can benefit.

After this was concluded it was decided to follow a suggestion of Dr. Olga Taussky and to develop the lectures given there into a book entitled "Survey of Numerical Analysis." Unfortunately, for various reasons not all the speakers who took part in the program participated in the development of the book, and there are some gaps.* In order not to affect the unity of the program, it was decided not to attempt to fill these gaps by including new contributions.† However, ample material is included for an introductory course, as well as representative chapters for advanced courses in numerical analysis and in supporting mathematics.

The authors are grateful to both organizations for the opportunity to present their ideas orally, and to their teachers, colleagues, and pupils for help in the later development.

Activities of Numerical Analysts

It is appropriate to discuss briefly what the activities of a numerical analyst should be. In addition to considering the exploitation of

* Several of the gaps have been covered by excellent monographs which have appeared recently. They cover, for example, such subjects as asymptotics, computability and unsolvability, initial-value problems, and linear programming.

† We note that Dr. Walter Gautschi and Dr. Werner C. Rheinboldt, who took part in the repetition of the Training Program (which took place in 1959, under the direction of Dr. Philip J. Davis), collaborated with Prof. H. A. Antosiewicz on Chapters 9 and 14.

automatic computers in new areas, he should be concerned with the solution of classes of problems: e.g., the solution of systems of linear equations, or the solution of ordinary differential equations. As well as reexamining old methods in the light of available equipment, he should be devising and evaluating new methods. Since, in general, it will be impossible for him to give the methods a complete theoretical examination, he should carry out controlled computational experiments, in which, for instance, he compares the observed errors with his theoretical estimates for realism. These experiments should be recorded and analyzed. Finally, he should construct and discuss "bad examples."

Such material, when combined with the experience of computers and the intuition of the customer, will be invaluable when the methods are being applied in practice, beyond the regions in which they are secure in the sense of classical mathematics.

The Education of Numerical Analysts

Informal teaching of the use of computers and of numerical analysis can begin at a very early stage. Formal teaching is appropriate whenever a reasonable background in the calculus and matrix theory is achieved—usually in the junior year. The contents of Chapter 3 and the first part of Chapter 8 are appropriate in a basic science curriculum. However, in view of the current tendency to abstraction, it may be necessary to incorporate them in the basic numerical analysis course. This course should include, in addition, most of the contents of Chapters 1, 2, 4, 5, and 6. We have covered this material in a two-quarter course, with three lecture hours per week and appropriate machine time.

We believe that there should be no division between theoretical and practical numerical analysis, and that a lecture without numerical examples is a lecture wasted. The instructor should have had recent machine experience and the supervision of practical work should, as far as possible, not be delegated. The following general advice was given by Prof. G. Pólya* to prospective high school teachers: "Acquire, and keep up, some aptitude for problem solving." This is particularly relevant here, and to it we would add the further qualification of experience in making examples.

Our worked examples and problems have an academic flavor, but this is mainly for brevity. They can be dressed up by the instructor according to his taste; for instance, he can relate the calculations of the zeros of Bessel functions to the eigenvalues of a differential equation and to the frequencies of vibrations of a drumhead. It is not possible

* G. Pólya, On the Curriculum for Prospective High School Teachers, *Amer. Math. Monthly*, vol. 65, pp. 101–104, 1958.

to include in a survey significant case studies in, for example, reactor engineering, astrophysics, or geophysics. Fortunately, however, monographs on such topics are becoming available.

Only in exceptional circumstances will teaching institutions be able to provide computers and computer organizations at the level of the best of the governmental and commercial installations. Generally, therefore, we recommend that students get experience in such centers as soon as they have completed the basic course. After this they will be in a better position to appreciate advanced courses. Since the practicing numerical analyst meets problems from many different areas, one-quarter courses, such as could be based on the material in the later chapters, are appropriate rather than more extensive treatments of special topics.

Finally, in view of the rapid developments in the field, students must be encouraged from the beginning to get acquainted with the periodical literature; for this purpose we have given ample references in the text and in the problems. The need for critical reading should be emphasized.

Remarks

In a composite work of this character, complete uniformity and freedom from overlap is almost impossible to maintain. The known inconsistencies in notations and terminology should not disturb the reader, and the repetitions are to his advantage. We hope that the errors and inaccuracies which have been overlooked will not be troublesome.

In the last decade, the electronic engineers have increased the power of our computers about a thousandfold; unfortunately there has been no comparable development in the relevant mathematics. We hope that this "Survey" will aid such a development; our views on this point are elaborated in Chapter 1. Although it may well be that the greatest contribution of automatic computers will be outside of the physical sciences, there is no doubt that a thorough grounding in mathematics and numerical analysis is the best initial training for those concerned with the use of computers if they are to avoid the many logical and arithmetic perils which await those who use their machines formally and uncritically.

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Motivation for Working in Numerical Analysis*

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1.1 Introduction

The profession of numerical analysis is not yet so desirable that it is taken up by choice; indeed, although it is one of the oldest professions, it is only now becoming respectable. Most of those who are now working in this field have been more or less drafted into it, either in World War I or in World War II, or more recently. The question at issue is, Why have they stayed in this field and not returned to their earlier interests?

The answer is that numerical analysis is an attractive subject in which mathematics of practically all sorts can be used significantly and from which many branches of mathematics can benefit. We call attention here to the applications of functional analysis by the Russian school led by Kantorovitch [1]. (For a survey of some Western work see Collatz [1*a*]; see also Altman [90].) In another direction we recall the developments in analytic number theory by Lehmer and Rademacher which followed MacMahon's computations of $p(n)$ for Hardy and Ramanujan [2]. We note here the contribution of machines to a problem on rearrangements in real variable theory due to D. H. Lehmer [91], to the theory of finite projective geometries and related fields by Hall and his

* This is a slightly revised and extended version of the article, with the same title, which appeared in *Comm. Pure Appl. Math.*, vol. 8, pp. 97–116, 1955, and which was reprinted in "Transactions of the Symposium on Computing, Mechanics, Statistics and Partial Differential Equations," F. E. Grubbs, F. J. Murray, and J. J. Stoker, eds., Interscience Publishers, Inc., New York, 1955. We are grateful to the publishers for permission to reproduce this here. A translation of this article into German, by Prof. Dr. E. Kamke, appeared in *Jber. Deutsch. Math. Verein.*, vol. 58, pp. 11–38, 1955; and a Russian version has appeared in *Matematicheskoe prosveshchenie*, vol. 1, pp. 75–86, 1955, and vol. 2, pp. 97–110, 1956.

collaborators (see Chap. 15), to a problem of Taussky [122] in the theory of sequence spaces by Kato [101], and to complex-function theory by Kreyszig and Todd [93] and Kusmina [94].

Before proceeding to a discussion of some individual topics in numerical analysis, some general remarks are in order. We have, on various occasions, distinguished between classical and modern numerical analysis, the latter being material required in connection with the exploitation of high-speed automatic digital computing machines. It now seems desirable to recognize ultramodern numerical analysis, which may be specified as adventures with high-speed automatic digital computing machines (see [50, 51]). There are, of course, no sharp boundaries between these parts of the subject, and there is room for development in the classical phases as well as in the newer areas.

In distinction to the deliberate explorations contemplated in ultramodern numerical analysis, there is much routine work in numerical analysis which must necessarily be of an experimental or empirical nature. It is just not feasible to carry out rigorous error estimates for all problems of significant complication; it is necessary to place considerable reliance, on the one hand, on the experience of those familiar with similar problems and, on the other, on the good judgment of the setter of the problem. To justify this remark, we consider three examples. The solution of systems of 20 or more first-order differential equations is being handled regularly. To see the complication of theoretical error estimates [in which the fact that all numbers handled are finite (binary) decimals is disregarded], we refer to Bieberbach [3]. The complication of a stability analysis in a system of 14 equations is evident from a study carried out by Murray [4]. Again, the extent of a complete error estimate for the problem of matrix inversions is familiar from the work of von Neumann and Goldstine [5, 5*a*] and Turing [6]. Finally, there are the analysis of the triple-diagonal method for determining the characteristic roots of a symmetric matrix by Givens [7, 7*a*] and the analysis of the Jacobi diagonalization method by Goldstine, Murray, and von Neumann [26].

What the numerical analyst has to do is to be aware of the precision of results obtained from, for instance, the conformal mapping of an ellipse on a circle by a certain process and, from these results, to extrapolate to cases of regions of comparable shape. On the one hand, he has to examine general error analyses for their realism by comparison with cases where the explicit, exact results are known. On the other hand, he must devote time to the construction and study of bad examples so as to counteract any tendency to too much extrapolation. For a preliminary discussion of matrix inversion in the last two directions, we refer to Newman and Todd [95] and to Todd [76, 77].

The main part of this chapter is devoted to a discussion of some topics in numerical analysis which appear attractive. These have been chosen, among those with which the author is familiar, to point out some of the techniques of the subject and to indicate some of the mathematicians who have made distinguished contributions in the field. In addition, the choice has been controlled by the author's opinion that separation between theoretical and practical numerical analysis is undesirable. The practicality of some of the techniques used is illustrated by computations of the radiation from a simple source which is reflected from a Lambert plane, recently carried out by Henrici [8], where the ideas of Secs. 1.3 and 1.6 were used.

1.2 Evaluation of Polynomials

What is the best way of computing polynomials, for instance,

$$f(x) = a_0x^n + \cdots + a_{n-1}x + a_n,$$

for a series of values of x, not equally spaced? (In the case where the values of $f(x)$ for a series of equally spaced values of x are required, building up $f(x)$ from its differences might be the most convenient.) The usual answer is to suggest the recurrence scheme:

$$f_0 = a_0,$$
$$f_{r+1} = xf_r + a_{r+1}, \qquad r = 0, 1, \ldots, n-1,$$

which was known to Newton but is usually ascribed to Horner [9]. In this way we get $f(x)$ by n additions and n multiplications. Is this the best possible algorithm? Consider an alternative, in the case of

$$f(x) = 1 + 2x + 3x^2.$$

If we proceed as follows:

$$2x,\ x^2,\ 3x^2,\ 1 + 2x + 3x^2,$$

we need 3 multiplications and 2 additions compared with the 2 multiplications and 2 additions needed in applying the above algorithm; thus

$$3x,\ 3x + 2,\ x(3x + 2),\ x(3x + 2) + 1.$$

This problem was formulated as one in abstract algebra by Ostrowski, and he showed [9] that the above algorithm was indeed the best for polynomials of degree not exceeding 4. A different approach was made recently by Motzkin [10] (see also Belaga [98]). Not restricting himself to purely rational processes, he showed that algorithms which are