



FORMAN S. ACTON





NUMERICAL METHODS THAT WORK

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Forman S. Acton

PROFESSOR EMERITUS OF COMPUTER SCIENCE PRINCETON UNIVERSITY



THE MATHEMATICAL ASSOCIATION OF AMERICA

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PREFACE-90

As I think about the reprinting of this numerical methods book, now twenty years old, I consider what Time and the PC have done to its message. In 1970 computers were 'large'; scientists and engineers used them in laboratories; numerical software for solving various types of equations could be borrowed from a friend but was not very reliable and was poorly documented. In 1989 computers have moved into the office and into the spare bedroom of the engineer's home. Numerical software is widely available but is not very reliable and is poorly documented. Of course Newton's Method is 20 years older but it seems to be bearing up well. Indeed, with the advent of programs that do *analytic* differentiation, his method has become even more attractive.

The big change has been to place the capacities of the large 1970 computer in the hands of many who previously would have had to seek far and perhaps borrow time on someone else's machine. But access to bigger memories and faster cycle times have not changed the useful algorithms; they have merely increased the sizes of the problems that now seem feasible— almost always *linear* problems. And linear algebraic algorithms and software were, and still are, the one reasonably reliable group of 'black-boxes'. They were good enough in 1970 so that most computer users were not going to write their own; one simply had to know why one *needed* to solve a system of 100 linear equations—a question all too often ignored then, and now! But

that important question lies outside the scope of this book (and the competence of its author). He has here merely raised the minatory finger—and having writ, moves on.

New tools have appeared: symbolic mathematical packages like Maple and Mathematica* that can reduce the drudgery (and increase the accuracy) of expanding complicated expressions into Taylor series. But they do not address questions about whether expansion will be a useful tactic—and if you have never before used one of these systems you will spend much more time learning how than you would expanding the immediate problem by hand. (Don't buy a chainsaw if you only have one sapling to cut! I assume that anyone reading this book is not about to tackle a forest.)

Since 1970 the Bulirsch-Stoer algorithm, mentioned briefly herein, has achieved a small but firm place among the ordinary differential equation integrators but its enthusiastic promoters have yet to produce an exposition that could fairly be included in a book at this level. Indeed, even to more sophisticated audiences they recommend it as a black-box, saying, in effect. "Try it—you'll like it!" I have been burnt by too many black boxes to take that position. Of course I regularly use other peoples' software, but if I can't fix a numerical algorithm, I won't use it. And since I haven't used B-S, I'm in no position to urge it on the public, however felicitous it may be.

Partial differential equations at a realistic algorithmic level require a book of their own. I only attempt to show the 'flavor' of the classical, still useful Finite Difference technique and point out some of the issues that must be addressed. For some partial differential equations Finite Elements, not even mentioned before, have certainly established themselves as a serious alternative to Finite Differences (tho, in my opinion, will never eliminate them) but to add Finite Elements now would have considerably lengthened the book and raised the expository level without enabling the reader to use them even on simple problems.

My doleful conclusion is that REAL algorithmic progress during the last twenty years has been principally in specialized areas that the student will wisely avoid in a first course. But from the student's point of view that means he really doesn't have to master a lot of new esoteric material. It's the best of worlds; it's the worst of worlds.

TO THE INSTRUCTOR

This book discusses efficient numerical methods for the solution of equations algebraic, transcendental, and differential—assuming an electronic computer is available to perform the bulk of the arithmetic. I wrote it for upper-class students in engineering and the physical sciences—men who have had calculus and a first exposure to differential equations. More importantly, I wrote it for students whose motivations lie in the physical world, who would get answers to "real" problems. This intended audience shapes both the content of the book and its expository method.

My principal concern has been the proper matching of the tool to the job. Conversely, it has not been the indoctrination of the student into the beauties of analysis—numerical or otherwise. Students with motivations from the physical world are best led from the specific example to the general method. They rapidly become impatient with the development of a logical superstructure for which they have seen no practical use. An average junior in engineering at Princeton will follow an unmotivated mathematical derivation or proof for about 20 minutes before writing it off as "some more mathematical Mickey Mouse."

When a student's principal thrust is to solve problems, the author and instructor should talk principally about how problems are solved. Methods can be introduced with geometric, sometimes heuristic, arguments. Initially at least, their justification is that they work. The student uses these methods, achieving a sense of power in being able to solve problems that his mathematics courses seem to have ignored. Then he tries a problem on which the method falters: a singularity appears, or too many significant figures disappear, or a debilitating instability arises. Now, *and not before*, is the student willing to delve into the deeper structure of the numerical method—convinced that its established utility can be retrieved and broadened only by such an effort. At this point his calculus training can be called into necessary play; at this point he can be shown the proof, especially a constructive proof. But at no point can he be expected to enthuse over, or even to tolerate, the systematic derivation of 17 quadrature formulas via some finite difference operator calculus. He doesn't need the 17 quadrature formulas, and he doesn't need to know how to derive them—elegantly or at all.

The book is divided into two parts, either of which could form the basis for a one-semester course in numerical methods. Part I discusses most of the standard techniques: roots of transcendental equations, roots of polynomials, eigenvalues of symmetric matrices and so on. This material can profitably be learned at the sophomore or junior level and, indeed, with the increasing availability of automatic computing equipment on American campuses, much of it is already diffusing into the standard freshman and sophomore courses in mathematics, physics, and engineering.

Part II cuts across the basic tools, stressing such common problems as instabilities in extrapolation, removal of singularities, loss of significant figures, and so on. It also introduces some of the methods that are useful with the larger problems associated with partial differential equations. At Princeton many students take the material of Part II as their first formal course in numerical methods—having absorbed the earlier material largely by osmosis. Some remedial reference to Part I is occasionally needed, but surprisingly little has been necessary in the last two years. The material of Part II is normally taken at Princeton by juniors and seniors.

I have tried to write a readable book. Clarity in presenting major points often requires the suppression of minor ones, at least temporarily. Thus the trained mathematician will encounter statements that are "incorrect" in the sense that all the qualifications and exceptions necessary to make them precise are not set forth nearby. The instructor may wish to warn the students about these inaccuracies and even to supply the lacunae, but here I would recommend caution. An excess of fleshy detail before the student has a firm skeleton on which to hang it is a burden that frequently will bring down the entire structure, leaving a heap of rubble that has neither beauty nor utility. Exceptional information ought to be supplied the *second* time through the subject, or when the student asks for it. The curious student who wants more complete discussions may be referred to the book by Ralston with a warning that it is written for the first-year graduate student. One topic is largely missing: formal error analysis with its emphasis on inequalities leading to bounds on approximations. I firmly believe such an analysis should be delayed until at least the third time through a numerical method. The student oriented toward results quickly discovers that the expedient way to test his methods is to run them again at half the interval and with slightly perturbed input data. Not that this expediency will catch all inadequacies in his finite difference approximations, but it will deal with a far greater percentage of them than will any formal error analysis.

I have not usually tried to prove convergence of any iterative process. It is a commonplace that numerical processes that are efficient usually cannot be proven to converge, while those amenable to proof are inefficient. Again my plea is insufficient pertinence to the student's purpose. The best demonstration of convergence is convergence itself. Judicious introduction of these two topics at the few places where they produce insight may be desirable, but they are so formidable in typographic appearance that all but the most docile students usually skip them. I prefer to leave their formal presentation to the instructor's discretion.

Finally, pedagogical expedience strongly suggests that the teaching of programming of digital computers be clearly separated from the teaching of numerical methods for solving problems, at least at the elementary levels. Any person who has mixed the two realizes how hopelessly the two sets of difficulties become intertwined both in the minds and in the practice of the students. At the advanced level, to be sure, the interaction between programming techniques and numerical algorithms is a fruitful study, but the sophomore should be exposed to fruitful studies in homeopathic doses! We recommend that the ability to write simple programs in FORTRAN, PL/1 or ALGOL be a prerequisite to this course, while access to a reasonable computer is almost a necessity.

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TO THE STUDENT

I hope you like to formulate physical phenomena into equations and then solve those equations to see how well your formulations actually predict experimental results. It is for such people that I wrote this book. But if you have tried this fascinating game, you have realized that solving the equation is frequently harder than getting it in the first place.

The complexities of theoretical formulations soon frustrate our ability to solve their equations analytically, and numerical solution methods—when performed by hand—often require days of laborious arithmetic. Thus, in the past, engineers, always under pressure to produce working devices quickly, have tended to avoid theoretical formulations. To solve anything quickly before the advent of the electronic computer meant to solve it analytically, and this usually required analytic simplification to the point where the answers had only a remote connection with the original problem. Experiment with an actual device was much quicker.

In the 1940s a big change occurred in some sectors of Engineering. Atomic explosions and jet aircraft required experiments that were no longer simple, cheap, or quick. Five years and millions of dollars were involved before a new idea for a jet engine could be pronounced successful, and the costs of an atomic test were not measured merely in money. Theoretical investigation suddenly had become a necessity for the engineer instead of a pleasant pastime. In 1950, Von Neumann's computer opportunely appeared, solidly establishing the theoretical investigation as a practical developmental tool, sometimes *the* practical tool, and nothing has been the same since.

The incorporation of numerical methods into the engineering curriculum is only now taking place, and there is still considerable discussion over how it should be done. Thus, if you are a student, you are probably coming into an upperclass course in Numerical Methods after having had the classical exposure to calculus and differential equations that has been pretty much standard since Newton (but without Newton's numerical experience!) or so I have assumed while writing this book. (If anybody asks me, I'll be glad to suggest a quite different curriculum that I feel would be far preferable for the final quarter of the twentieth century.)

Having disposed of the question "Why learn about numerical methods?" let me now get around to the equally important question of how to learn about them. I shall be brief.

Numerical equation solving is still largely an art, and like most arts it is learned by practice. Principles there are, but even they remain unreal until you actually apply them. To study numerical equation solving by watching somebody else do it is rather like studying portrait painting by the same method. It just won't work. The principal reason lies in the tremendous variety within the subject. By contrast, analytic solution methods work for very restricted classes of problems. Thus we know how to solve ordinary differential equations analytically, provided they are linear and with constant coefficients! Let them have variable coefficients, and we become quite unsure of ourselves. If any nonlinearity creeps in, you might as well give up. But all three kinds of ordinary differential equations can be solved by numerical methods—provided, of course, that a solution exists. Thus it would be quite surprising if one numerical method succeeded everywhere—and no single method does!

The art of solving problems numerically arises in two places: in choosing the proper method and in circumventing the main road-blocks that always seem to appear. So throughout the book I shall be urging you to go try the problems—mine or yours.

I have tried to make my explanations clear, but sad experience has shown that you will not really understand what I am talking about until you have made some of the same mistakes that I have made. I hesitate to close a preface with a ringing exhortation for you to go forth to make fruitful mistakes; somehow, it doesn't seem quite the right note to strike! Yet, the truth it contains is real. Guided, often laborious, experience is the best teacher for an art. If all you desire is a conversational knowledge of an art, you've chosen the wrong subject, the wrong author, and just possibly the wrong profession. It is one of the minor paradoxes of our language that, even in the 1970s, you learn how to solve real problems only by getting your hands dirty with rational numbers—although rational problems can frequently be solved only with real numbers. Good luck !

AFTERTHOUGHTS

The students in my Numerical Methods course usually have been Juniors—with a sprinkling of graduates and the occasional rather sophisticated Sophomore. Mostly they have been Engineers and Scientists. (Mathematicians at Princeton are proudly Pure while most Computer Scientists find an obligatory decimal point to be slightly demeaning.) Thus the student interest has centered on solving 'typical' physical problems that in practice devolve to simplified versions such as those treated in the text. Since some instructors have requested more exercises I have included some more below.

My recent practice has been to go rapidly through the first 6 chapters in as many weeks with weekly computation laboratories in which simple (pencil and pocket-calculator) problems are worked with an instructor present to get people out of mudholes onto productive paths. (These sessions are partly remedial as at least half of my students have had some exposure to these early topics in a first computer programming course that contained considerable numerical methods.)

In the second half of the semester I cover topics from the rest of the book according to the perceived class interests but the computational homework has been devoted entirely to one half-term project—each student's problem being unique. I feel strongly that somewhere in the undergraduate scientific curriculum the student should be asked to work a problem to which he does not know the answer and for which the answer, when found, should not proclaim its correctness. In most underclass courses the answers to the exercises are known *a priori*: they are in the back of the book or they turn out to be π or $\sqrt{2}$ —or one's roommate did the problem last term. For such problems the effort goes entirely into *getting* the answer. But in realistic engineering problems somewhere between 50 and 90 percent of the effort goes into *verifying that the 'answer' obtained is, indeed, correct*. The student needs this kind of experience at least once, somewhere, and I choose to supply it here.

A problem type that has been very effective for these purposes is the preparation of an efficient computer *function* (i.e., a working, thoroughly debugged program) for an integral like

$$H(b) = \int_0^\infty \frac{e^{-bx}}{\sqrt{x(1+x)}} dx.$$

For large b an asymptotic series is useful; for small b a singularity has to be propitiated, analytically, before a series in b is possible—and these two approaches leave a gap that the student has to struggle to fill. One of the ground rules is that numerical quadrature is *not* to be part of the final function (too slow) although it is a necessary tool during the development. Likewise, covering the gap by interpolation in a large stored table lies outside the aesthetic framework of the exercise, although I have reluctantly accepted it for part credit when submitted as a last-ditch effort by a weak student. A mature mathematician can perform this exercise in a couple of afternoons, but a student often needs a half-semester of a course, even with considerable help. Weekly conferences with the instructor are essential; without them, there is the danger that work either is postponed into impossibility or proceeds forever down ultimately unproductive paths.

There is a whole family of similar integrals that can be assigned; generally

$$G(b) = \int_0^\infty \frac{e^{-bx^j}}{x^k (1+x^l)^m} dx$$

with

$$j = 1, 2$$
 $k = 0, 1/2$ $l = 1, 2$ $m = 1/2, 1$

that offer varying degrees of difficulty so that the problem can be tailored to the student's abilities—or ambitions. In addition to the techniques covered in the book, most of these integrals can be evaluated efficiently by rather sophisticated recurrences. When time has permitted I have derived the recurrence for the integral of page 261*—thereby tempting the better student to explore this new tool for his gap-covering algorithm.

Tests and examinations

I have usually given two 50-minute tests and a final 3-hour examination. These, together with observations available from the labs and weekly project conferences have provided a more-than-adequate basis for grading. The tests have been 'closed book' except for Abramowitz & Stegun and a pocket calculator — neither of which are usually necessary but knowing that they will be available usually keeps the students from spending time memorizing formulae. Hopefully they will have concentrated on strategic algorithmic principles. Here is a 50-minute test that is difficult to do well but one that provides good opportunities for exhibiting mastery of the course concepts.

Test

1. It is necessary to compute the sequence of 50 functions

$$F_k(b) = \int_0^1 e^{bt} t^k dt \qquad k = 0, 1, \dots, 49$$

for various b that are not known at the time you must write the computer program. Integration by parts gives the recurrence

$$bF_k(b) + kF_{k-1}(b) = e^b$$
 $k = 1, 2, ...$

from

$$F_0(b) = (e^b - 1)/b$$

*Run

$$I_{n-1} = I_n + cK_n/(2n)$$
 $J_{n-1} = (2nJ_n + cI_{n-1})/(2n-1)$ $K_{n-1} = K_n + J_{n-1}$

from largish N down to 1, whence $F(b) = J_0/c/K_0$. The starting values of I_n , J_n and K_n are arbitrary but should not all be zero.

The recurrence is economical, if usable. For what values of (b, k) can the recurrence be used to deliver 10 significant figures (or 10 decimals, if you prefer) on a 13 digit machine?

2. a) How would you integrate

$$b\frac{d^2u}{dt^2} + \frac{a}{t}\frac{du}{dt} + u^3 = 0$$

from the initial conditions

$$u(0)=1 \qquad \frac{du}{dt}(0)=0$$

for various (a, b)?

- b) If the coefficient b is large (say, 1000), what effect will it have on your favored process?
- 3. A large number of peculiar quintic polynomials are to be solved for all their real roots that lie on the range (-10, 10). These polynomials are peculiar because the coefficient of their x^5 term is typically smaller than the other coefficients by at least a factor of 100. Five algorithms are listed below.
 - a) Write 2 or 3 sentences about each, explaining how it can be applied to this problem (if at all) and comment on its usefulness.
 - b) Give your recommendation for handling this problem—not necessarily from the list—and defend it.
 - 1. Forward-Backward Division
 - 2. Newton's Method
 - 3. Binary Chop
 - 4. Lin's Method
 - 5. Lehmer's (concentric circles) Method

Exercises

These exercises are intended to be performed with pencil, paper and a pocket calculator. Most are 'remedial' in the sense that, ideally, students taking this course should be able to do them in relatively short order—say, 5 to 20 minutes each—on the basis of prior experience. Since many lack that experience, I have given them in supervised laboratories where individual guidance is available before too much frustration sets in.

Precision Problems

1. How would you evaluate

$$\ln\sqrt{x+1} - \ln\sqrt{x}$$

for large x without losing significant figures? Compare your method with direct evaluation for x = 123456.7.

2. Find the behavior of

$$\ln\left[\frac{\sqrt{1+x^2}-x}{\sqrt{1+x^2}+x}\right]$$

- a) for large x
- b) for x near zero

and then suggest how the function should be evaluated.

3. Evaluate

$$w(x) = 1 + \frac{1}{2} \tanh x^2 - \cosh x$$

for x = 0.1

- a) as expressed here
- b) from a series expansion

Keep all arithmetic to 10 significant figures if possible. Where and how does error arise?

4. Consider evaluating

$$\frac{\cosh x}{2 - \cos x} \qquad x \ge 0$$

and then decide how you would solve for

$$\frac{\cosh x}{2 - \cos x} = 1 + \epsilon$$

for small ϵ .

- 5. How should one solve $\tan \theta = B$ for θ if B is greater than 10? Assume you do not have specialized tables.
- 6. Devise iterative computational algorithms for solving

$$\frac{\tanh x}{\arctan x} = b$$

for x when a) $b = s \operatorname{near} 2/\pi$ b) b is near 1

without serious instability or loss of significance. Estimate the range of applicability of your algorithms.

7. Consider the quadratic equation obtained by eliminating either the $\sin^2 x$ or $\sinh^2 y$ term from the equation pair

$$\beta = \sin^2 x + \sinh^2 y \qquad \beta = u^2 + v^2$$

$$\alpha \tanh^2 y = \tan^2 x \qquad \alpha = u^2/v^2$$

as a method for determining x and y when (u, v) are given. Where are the trouble spots? What has to be done to avoid significant figure loss? How many separate algorithms do you end up with via this approach?

8. Examine the limiting behaviors of

$$\frac{\sin x}{1 + \cos x}$$
 and $\frac{\sinh x}{\cosh x - 1}$

as x approaches zero (from each side).

Conformal mapping

[The student should have seen complex variables in their rectangular and polar forms, but no course in the subject is presumed. The instructor should do a mapping first—perhaps $z = \sin t$ using the first quadrant of t.]

9. Find the complex z-map of the figure under

$$z = \tanh t$$

$$\pi/2 \frac{100}{t}$$

labelling the critical points.

10. Consider the mapping from t to w of the figure in Problem 9 via

$$\sin w = \tanh t$$
.

Compare the final potential problem with the original one.

11. Devise an algorithm to evaluate a point w that corresponds to a *complex* value of t near $(0, i\pi/2)$.

Singularity removal

12. Find a series in b for

$$F(b) = \int_0^1 \frac{dx}{\sqrt{1 - bx^3}}$$
 (a)

when b is small. How many terms are needed to obtain approximately 8 significant figures when b is 0.5? For what ranges of b values is the series practical? Then transform

$$\int_0^1 \frac{dx}{\sqrt{1-x^3}}$$

to remove the singularity, sketch, estimate its value. Devise a method for evaluating $F(1 - \beta)$ when β is small. [*Hint*: Transform the dummy variable in (a) so that the parameter is in the *limit* rather than in the integrand. Then consider an integral that is related to the difference between F(1) and F(b).]

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