NUMERICAL METHODS FOR ENGINEERS AND SCIENTISTS

A students' course book

A.C. BAJPAI · I.M. CALUS · J.A. FAIRLEY

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PREFACE

This is a volume of programmes on numerical methods which is part of a course written for undergraduate science and engineering students in universities, polytechnics and other colleges in all parts of the world. Numerical methods are now included in the syllabuses for all such students and this book covers most of the work that these students are likely to require. The emphasis is on the practical side of the subject and the more theoretical aspects have been omitted. Numerical methods are, of course, closely linked to the use of the computer and several references will be found as to the suitability of various methods for programming on to a computer. As different programming languages are in use, the various techniques discussed have not, with one exception, been translated into computer programs, but, wherever appropriate, flow diagrams have been incorporated into the text. References have, however, been given to other books in which typical computer programs can be found. A list of these references appears on page 377.

When one is using numerical methods as a tool, the majority of the calculations would be done on a computer, as, except in a few simple cases, the amount of arithmetic involved is far too complicated to do any other way. However, when learning the subject there is nothing, in general, to be gained by taking very complicated examples or by carrying working through to a very large number of significant figures. Doing relatively simple examples manually does give the student an appreciation of what is involved and so the actual numerical working of many examples has been included.

If the reader has access to a calculating aid, such as a pocket calculator, it will be found very helpful. However, if not, it will often mean that the working can only be done to fewer significant figures or decimal places than is indicated. It is suggested, therefore, that, irrespective of the number of decimal places asked for, working is only done to such a number as can conveniently be obtained. Any points that consequently might not be obvious can still be followed from the working in the text.

The volume comprises three Units in which are grouped programmes on allied topics. Before reading a programme, the student should be familiar with the items listed under the heading of Pre-requisities at the beginning of each Unit. The programmed method of presentation has been used throughout and has many advantages. The development of the subject proceeds in carefully sequenced steps, the student working through these at his own pace. The active participation of the student is required in many places where he or she is asked to answer a question or to solve, either partially or completely, a problem. The answers to these are always given so that the student can check his attempt and thus obtain a continuous assessment of his understanding of the subject. Explanation of the material covered is given in greater detail than is often to be found in conventional style textbooks, especially at those points where difficulties are most likely to occur.

In places where units are involved, the S.I. system has been used. The standard practice of using italic letters for quantities, e.g., *C* for capacitance, has not, however, been followed as italic lettering is used for the answer frames. Where natural logarithms occur, the notation ln is used.

Where references are made to frames in the same programme, only the frame numbers are given. Where page numbers are quoted as well, this indicates that references are to frames in another programme.

Several references are made to our volumes on Mathematics for Engineers and Scientists. The details of these books are:

Mathematics for Engineers and Scientists, Volume 1.
A.C. Bajpai, I.M. Calus, J.A. Fairley Wiley, 1973.

Mathematics for Engineers and Scientists, Volume 2.
A.C. Bajpai, I.M. Calus, J.A. Fairley, D. Walker Wiley, 1973.

We have also referred to

Fortran and Algol
A.C. Bajpai, H.W. Pakes, R.J. Clarke, J.M. Doubleday, T.J. Stevens
Wiley, 1972.

In spite of careful checking by the authors, it is possible that the occasional error has crept through. They would appreciate receiving information about any such mistakes which might be discovered.

A debt of gratitude to the following is acknowledged with pleasure:

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The *University of London* and the *Council of Engineering Institutions* for permission to use questions from their past examination papers. These are denoted by L.U. and C.E.I. respectively.

John Wiley and Sons Ltd for their help and cooperation.

INSTRUCTIONS

Each programme is divided up into a number of FRAMES which are to be worked *in the order given*. You will be required to participate in many of these frames and in such cases the answers are provided in ANSWER FRAMES, designated by the letter A following the frame number. Steps in the working are given where this is considered helpful. The answer frame is separated from the main frame by a line of asterisks: ********. Keep the answers covered until you have written your own response. If your answer is wrong, go back and try to see why. Do not proceed to the next frame until you have corrected any mistakes in your attempt and are satisfied that you understand the contents up to this point.

Suggestion to the Reader

It is strongly recommended that you make use of a pocket calculator to help you with the arithmetic involved in the examples.

CONTENTS

UNIT 1 - Equations and Matrices

UNIT 2 - Finite Differences and their Applications

INTERPOLATION

NUMERICAL DIFFERENTIATION

NUMERICAL INTEGRATION

UNIT 3 - Differential Equations

FIRST ORDER ORDINARY DIFFERENTIAL EQUATIONS

SIMULTANEOUS AND SECOND ORDER DIFFERENTIAL EQUATIONS

PARTIAL DIFFERENTIAL EQUATIONS

UNIT 1
EQUATIONS and MATRICES

This Unit comprises four programmes:

(a) Basic Ideas, Errors and Evaluation of Formulae
(b) Solution of non-Linear Equations
(c) Simultaneous Linear Equations
(d) Matrices

Before reading these programmes, it is necessary that you are familiar with the following

Prerequisites

For (a): Differentiation, including the definition of a derivative in terms of a limit.

For (b): The binomial theorem, differentiation and Taylor's series for the main programme.

Maxima and Minima for APPENDIX A.

Partial differentiation and differentials for APPENDIX B.

Notation of determinants and algebra of complex numbers for APPENDIX C.

Taylor's series in two dimensions for APPENDIX D.

For (c): Evaluation of Determinants, matrix notation for linear simultaneous equations, including the augmented matrix, for the main programme.

Partial differentiation and differentials, the properties of inequalities of absolute values for the APPENDIX.

For (d): The algebra of matrices. The meaning of eigenvalues and eigenvectors and the analytical method of their determination.

Basic Ideas, Errors and Evaluation of Formulae

FRAME 1

Why Numerical Methods?

So far in your mathematics course, you have probably concentrated mainly on analytical techniques. Thus it is likely that you know how to find, for example,

$$\frac{d}{dx}\sin^2 3x \quad \text{and} \quad \int_0^{\frac{1}{2}\pi} x \cos 2x \, dx,$$

and also how to solve an equation such as

$$\frac{d^2y}{dx^2} - 2\frac{dy}{dx} - 3y = e^x$$

Again, you have probably met determinant and matrix methods for solving a set of simultaneous linear equations. So your reaction on encountering a book such as this may very well be - Why Numerical Methods? - or, perhaps, the even more fundamental question - What are Numerical Methods?

FRAME 2

When studying, for example, integration, you learn many techniques for integrating a variety of functions. Some of these techniques are integration by substitution, integration by partial fractions, integration by parts, etc. But whatever methods you learn, there are still many functions that you just cannot integrate. Two examples of such functions are e^{-x^2} and $\sin\sqrt{x}$. Again, when dealing with differential equations, anything slightly different from one of the few standard types of equation can lead to a situation whose solution is extremely difficult or even impossible by standard techniques. So you will see that we are sometimes very restricted in what we can do by purely analytical methods. However, don't get the impression that all your troubles will be over when you have finished this book. Some of them will be - for example, you will know how to find $\int_0^{0\cdot 2} e^{-x^2}dx$ but you will be no nearer to finding the indefinite integral $\int e^{-x^2} dx$.

FRAME 3

Turning for a moment to the solution of simultaneous linear equations, the use of Cramer's rule or of the formula $\frac{1}{\det A}\text{adj } A$ for A^{-1} does not present much trouble if, say, you have to solve three equations in three unknowns. However, if you have to solve fifty equations in fifty unknowns, such as can occur when dealing with space frames which are used in roof trusses, bridge trusses, pylons, etc., you are going to require some help with the arithmetic and for that help you will probably turn to a digital computer. This piece of equipment will almost certainly not use either of the two methods quoted above as the evaluation of determinants is a very time consuming process on a computer and 'time', where a computer is concerned, is simply another way of spelling 'money'. In such a situation, a numerical approach is adopted which, incidentally, is also purely mechanical in its operation.

FRAME 3 (continued)

Whilst on the subject of equations, there are many simple looking single algebraic equations that you would find very troublesome or impossible to solve analytically - for example, how would you set about solving the equation $e^x = 10 - x$? Such an equation can, however, be solved numerically, to any required degree of accuracy, with very little difficulty.

FRAME 4

Some problems which cannot be solved analytically do at least have an analytical look about them in the first place, for example, the equation $e^x = 10 - x$ and the integral $\int_0^2 e^{-x^2}\,dx$. However you may quite well meet a problem that is not even formulated in analytical terms. For example, suppose an experiment has been performed and a series of values of, say, the temperature θ of a body measured against a series of values of the time t. Thus the values of θ may be measured at intervals of one minute. Having performed the experiment, you may then be asked "What was the temperature after 5½ minutes?" or "At what rate was the temperature changing after 10 minutes?" You cannot use analytical means to answer questions such as these as the formula for θ in terms of t is not known. Again a numerical method is necessary to determine the answers to such questions.

FRAME 5

The following are some more examples of practical problems that require numerical methods for their solution:

The equation $\left\{\dfrac{\sin\alpha}{\alpha}\right\}^2 = \dfrac{1}{2}$ occurs in Fraunhofer diffraction. What value of α satisfies this equation?

The motion of a planetary gear system in a certain automatic transmission involves the equation $\sin\omega t - e^{-\alpha t} = 0$. What is the smallest positive value of t for given values of α and ω?

A certain column buckles when kL has the least positive value that satisfies the equation $\tan kL - kL = 0$. What is this value of kL?

The integral $\displaystyle\int_0^{x_0} \frac{x^4 e^x}{(e^x - 1)^2}\,dx$ occurs when obtaining the heat capacity of a solid by a method based on the vibrational frequencies of the crystal. What is the value of this integral for a given x_0?

The integral $\displaystyle\int_{\lambda_1}^{\lambda_2} \frac{1}{\lambda^5(e^{hc/\lambda kT} - 1)}\,d\lambda$ occurs in finding the fraction of total energy that is visible radiation of a black body. What is the value of this integral for given values of λ_1 and λ_2?

FRAME 6

Once a numerical method has been found for a particular type of problem, it can also be used for similar problems that do have analytical solutions. For example, the same numerical technique can be used for solving $x^2 - 2x - 14 = 0$ as for $e^x = 10 - x$. So your question now might be — If I can solve a greater variety of problems by numerical techniques than I can with analytical methods, why bother with the analytical techniques? This question has two answers:

(i) If an analytical technique exists, it is usually easier and more exact than the corresponding numerical method - for example, the easiest way of obtaining the solutions of $x^2 - 2x - 14 = 0$ is still by the use of the quadratic formula. But even this requires some method of evaluating $\sqrt{60}$.

(ii) Analysis forms the basis of many of the numerical techniques.

The conclusion we should draw is that both analytical methods and numerical methods have, in their own rights, their places in mathematics and that in any particular problem where there is a choice as to the method of solution, then the method chosen should be that which leads to the best combination of simplicity, speed and accuracy. As analytical methods have been considered in 'Mathematics for Engineers and Scientists, Vols. 1 and 2', by the present authors, this book will concentrate on numerical methods.

FRAME 7

Aids to Calculation

The majority of problems which are tackled by numerical methods involve a considerable amount of arithmetic. Some help with this arithmetic is obviously desirable and in most cases essential. Some of the aids available you will have already met - for example, mathematical tables and slide rules. These are useful tools when the number of calculations to be performed is limited and relatively few significant figures are required in the answers. Furthermore they are restricted to multiplication and division, being of no help for addition and subtraction. The number of significant figures obtainable with these aids can be increased by the use of more comprehensive tables, quoting quantities to more significant figures (e.g., six-figure instead of four-figure logs), and larger slide rules.

FRAME 8

Proceeding up the scale, so to speak, we next come to the mechanical desk calculator which is basically an adding and subtracting machine. However, as multiplication can be performed by a series of additions and division by a series of subtractions, many desk machines were modified so that they could carry out these operations either automatically or semi-automatically. The number of significant figures to which they could work was usually greater than is the case with either tables or a slide rule. Originally this type of machine was driven manually but later electrically driven models were introduced.

The mechanical type of desk machine has now been almost entirely superseded by electronic types and some of these are even programmable thus turning them into mini-computers. So rapid have been the recent

FRAME 8 (continued)

advances in this type of machine that electronic pocket calculators are now widely used.

FRAME 9

Useful as desk and pocket calculators no doubt are, they pale into insignificance when compared with a full-size digital computer. Not only is such a machine extremely fast but it can be given a whole set of instructions and left to get on with the job, whereas a desk machine requires constant attention. It is really the advent of the computer that has brought numerical methods into their own. Before computers were available there just was not the means of doing vast amounts of arithmetic at a reasonable speed. So although the numerical methods were there, their use was considerably restricted.

It may happen that there is more than one method available for solving a problem numerically. In that case the tendency these days is to use that method which is best suited to the computer.

FRAME 10

When applying numerical methods in actual practice, it is the more complicated type of problem (e.g., fifty simultaneous linear equations in fifty unknowns) that is liable to occur. However the methods used in the solution of such a problem are basically the same as those which can be used in much simpler cases (e.g., three simultaneous linear equations in three unknowns). As there is nothing to be gained when learning the actual methods by having very complicated problems, the examples used in these programmes to illustrate the methods will therefore be kept relatively simple.

If you have access to a desk machine or a pocket calculator you will find it a great help when working through the examples in this book. If, however, you haven't, you will still be able to do most of the working with the aid of a set of mathematical tables. This will mean that in some places you will only be able to work to a fewer number of significant figures with consequent loss of accuracy. In some examples you will find this loss of accuracy very marked. Even so, you will still be able to appreciate the techniques involved.

You may also have knowledge of a computing language. If so, then having learnt the technique of a numerical method, it will be a good idea for you to write a computer program for that method, and, if possible, get it run on a computer, using suitable data.

FRAME 11

Accuracy and Errors - Types of Error

Whenever calculations are performed there are many possible sources of error and errors will obviously affect the accuracy of the solution of a particular problem. Errors can be introduced in three ways:

(i) Mistakes made by the person carrying out the calculations,
(ii) The use of inaccurate formulae,
(iii) The use of inaccurate data, including the effects of round-off.

In the next few frames, we will have a look at each of these in turn.

FRAME 12

Theoretically, all errors made under the heading (i) shouldn't be there at all. But, as a certain gentleman once remarked: "To err is human ...." and the operator is, of course, human. However, in some cases he may be forgiven - if, for example, he is using a machine that has developed a fault which he cannot detect. Even so, such a fault is still going to affect the accuracy of his result.

Mistakes commonly made by a human operator occur when copying and when doing mental arithmetic. Two common copying errors are:

(a) the reversal of two digits, e.g. writing down 236 721 instead of 263 721, and

(b) the repetition of the wrong digit, e.g. 233 721 instead of 223 721.

It is obviously best to avoid such mistakes as these but as the chances are that you will still make some, it is advisable to take steps to, firstly, reduce the number that you make and, secondly, try to detect any that you do make as soon as possible.

To reduce the probability of making mistakes, it is very advisable to keep your computational work neat and tidy - and also legible. Furthermore try and arrange your work so that you have to copy numbers as few times as possible. To assist in detecting mistakes you should arrange to check your working wherever possible - not by repetition but by some independent process. How this can be done in certain cases will be indicated later.

In some types of work, mistakes are automatically taken care of. This does not mean, of course, that you shouldn't take care not to make them as they can still cause you to waste time.

FRAME 13

In the case of (ii), an inaccurate formula may arise due to chopping off an infinite series after a finite number of terms. For example, this is done when Simpson's rule is obtained by the use of Taylor series. $f(a - h)$ and $f(a + h)$ are expanded in powers of h but all terms involving powers greater than the second are dropped. An error introduced in this way is known as a TRUNCATION ERROR.

FRAME 14

A truncation error such as that described in the last frame leads to an approximate formula being used instead of an exact one.
Differentiation gives us another example where a true formula may be replaced by an approximate one. As you know, if $y = f(x)$ then the value of $\frac{dy}{dx}$ at the point $x = a$ is given by the formula

$$\frac{dy}{dx} = \lim_{h \to 0} \frac{f(a + h) - f(a)}{h}$$

Assuming h is small, $\frac{dy}{dx}$ is given approximately by the formula

$$\frac{f(a + h) - f(a)}{h} \qquad (14.1)$$

FRAME 14 (continued)

the accuracy increasing as h is decreased. To illustrate this, if

$$y = \frac{e^x}{x}, \quad \frac{dy}{dx} = \frac{x-1}{x^2}e^x \quad \text{and so, when} \quad x = 2, \quad \frac{dy}{dx} = 1{\cdot}8473.$$

Now use the formula (14.1) to find approximate values for $\frac{dy}{dx}$ when $a = 2$ and h is, in turn, 0•2, 0•1, 0•05, 0•01.

****

14A

2•038, 1•941, 1•892, 1•85.

FRAME 15

As we have already observed from our work on calculus, the result obtained always becomes better as h is decreased. At least it does theoretically. Practically there are certain other snags which may upset the apple cart, as will be seen later. You will also find later that many numerical methods involve the choice of an h (Simpson's rule is another example) and that when this is the case, the smaller it is, the better. However, there are other points to be noticed in connection with the results obtained in 14A, and we now come to errors introduced due to the use of inaccurate data [(iii) in FRAME 11].

When calculating the value of $\frac{dy}{dx}$ as given by the formula (14.1), you had to evaluate

$$\frac{\frac{e^{2\cdot2}}{2\cdot2} - \frac{e^2}{2}}{0\cdot2}$$

for the case when $h = 0{\cdot}2$. What aids did you use in evaluating this expression?

****

15A

Almost certainly you used exponential tables for $e^{2\cdot2}$ and e^2. The division by 2•2 you may have carried out on a desk or pocket calculator, by logs, on a slide rule or without any such aid.

Division by 2 and 0•2 and also the subtraction you probably did mentally.

FRAME 16

Accuracy and Errors — Round-off

Taking first the values of $e^{2\cdot2}$ and e^2 from (as we did) exponential tables to four places of decimals, the figures 9•0250 and 7•3891 are obtained. It is, of course, extremely unlikely that these are the exact values of $e^{2\cdot2}$ and e^2. They are almost certainly subject to ROUNDING ERRORS. These occur whenever a number is quoted correct to so many decimal places or significant figures, the quoted figure being thus not quite the true value. Various questions then arise such as:- What effect do such errors have on the result of the calculation? Are any other numbers in our original expression subject to error in this way? If so, what effect will this have on the result? Are any more round-off errors likely to occur during the course of the calculation?
