

Numerical Solution of Ordinary and Partial Differential Equations

BASED ON A
SUMMER SCHOOL HELD IN OXFORD
AUGUST—SEPTEMBER 1961

L. FOX M.A., D.Sc.

Director, Oxford University Computing Laboratory

PERGAMON PRESS

OXFORD · LONDON · NEW YORK · PARIS

1962

PREFACE

The Oxford University Computing Laboratory had its first Summer School, in collaboration with the Delegacy for Extra-Mural Studies, in September 1960. Some eighty representatives of government, industry, universities and technical colleges attended a two-week course on computational methods in linear algebra and differential equations. The material was rather introductory, but the success of the school was sufficiently encouraging to warrant a further venture in 1961.

We decided to concentrate on differential equations, and to try to supplement lectures on general techniques with discussion of some difficult particular problems, especially involving partial differential equations, which are the everyday concern of certain government, industrial and research departments. I felt that my colleague Dr. D. F. Mayers and myself could cover reasonably the topics of ordinary differential equations, integral equations, and an introduction to partial differential equations, but that lectures on practical problems in partial differential equations should be given by those who are actually solving them.

My requests for assistance met with prompt and very generous response. Dr. J. Corner (Atomic Weapons Research Establishment, Aldermaston) was glad to "have a platform" for the dissemination of recently declassified work of his department, and Dr. J. Howlett (United Kingdom Atomic Energy Authority, Harwell) also demonstrated his enthusiasm for co-operation between university and industry. In fact Howlett and Dr. J. Armstrong (A.W.R.E.) helped in the construction of the programme, particularly for the last part of the course.

I subsequently enlisted the willing help of Dr. J. Maccoll (War Office, Fort Halstead), the Meteorological Office (Bracknell), the Central Electricity Generating Board (London), the Computing Unit of London University, and Dr. H. Motz (Oxford University Engineering Laboratory), and the final programme listed the following 17 lecturers:

A.W.R.E. (Aldermaston): A. E. Glennie, N. E. Hoskin, B. W. Pearson, L. H. Underhill, L. M. Russell, J. B. Parker;

U.K.A.E.A. (Harwell): M. J. D. Powell, A. R. Curtis, I. C. Pyle; (Winfrith): I. C. Pull;

W.O. (Fort Halstead): D. S. Butler;

C.E.G.B. (London): Miss J. E. Walsh;

M.O. (Bracknell): E. Knighting;
London University: R. A. Buckingham,
O.U. Engineering Laboratory: H. Motz;
O.U. Computing Laboratory: L. Fox, D. F. Mayers.

So far this was just a course of lectures, but then Motz and Howlett suggested that the material should be published, and Captain I. R. Maxwell routed a very reluctant editor with the promise of publication only four or five months after receipt of copy. Again there was no hitch. All the manuscripts were produced by the date requested, and proofs began to arrive on the editorial desk almost before the expiration of the last breath of relief for the ending of a successful course.

The material of the first three parts covers the numerical solution of ordinary differential equations, integral equations, and partial differential equations of quasi-linear form. We have tried to include, either fully, briefly or by reference, all the important known facts and techniques, and have indicated what is not known, what we would very much like to know, and what current research is in progress. Throughout we have kept the electronic computing machine firmly in mind, but noting that the importance of numerical analysis has increased, rather than declined, with the advent of this instrument. Most of the techniques are therefore evaluated from the standpoints of accuracy, convergence and stability (in the various senses of these terms) as well as ease of coding and convenience of machine computation.

The material is fairly advanced, in the sense that we have tried to reach here the frontiers of knowledge in the relevant fields, but the style of writing is not that of professional mathematicians. We have written for scientists who have problems to solve, and who want to know what methods exist, why and in what circumstances some are better than others, and how to adapt and develop techniques for new problems. The mathematics is by no means ignored, but long and difficult proofs, for instance of the convergence of finite-difference processes to the true solution, are often sketched and not given, except by reference, in great and rigorous detail. The budding numerical analyst, however, should also benefit from this book, and will certainly find some topics for valuable research. The first three parts, in fact, could be used not only by practical men but also by students, though a preliminary elementary course would assist the reading.

The last part, on practical problems, uses and develops the techniques described earlier for the treatment of problems of the greatest difficulty and complexity, which tax not only the best machines but also the best brains. Much of this work is very new, containing frequent reference to "recent unpublished work". The first 300 pages, in contrast, are largely expository, though we have summarized the recent literature and presented in new ways

some older results and methods, and some of the work on integral equations is new.

The expository sections include ~~our own~~ versions of some of the material found in previous books, particularly those by Collatz (*Numerical Solution of Differential Equations*, English translation by P. G. Williams, Springer, 1960), Milne (*Numerical Solution of Differential Equations*, Wiley, 1953), Richtmyer (*Difference Methods for Initial-value Problems*, Interscience, 1957) and Forsythe and Wasow (*Finite-difference Methods for Partial Differential Equations*, Wiley, 1960). Generally we have concentrated a little more than these authors on practical and computational details, a little less on rigorous analysis, and we have learnt much from all of them. I hope that our selection of topics will prove to be soundly based, that at least some of our readers will be stimulated to study the more advanced parts of these and other texts, and that, through personal defect and shortage of time, the number of mistakes in fact and principle will not be prohibitively large.

I am deeply indebted to all the lecturers, and particularly to my colleague Dr. Mayers, who bore with me the brunt of the first week's lecturing; to the captive audience, who contributed to this book in no small measure both by silent and spoken interest; to the Extra-Mural Delegacy, who captured the audience; to my secretary, Miss Olive Moon, who typed with great accuracy some two-thirds of the text from manuscript which nobody else could read; and to the Pergamon Press, who fulfilled their function with uncommon skill.

Oxford

L. Fox

PERGAMON PRESS INC.
122 East 55th Street, New York 22, N.Y.

PERGAMON PRESS LTD.
Headington Hill Hall, Oxford
4 & 5 Fitzroy Square, London, W.1

GAUTHIER-VILLARS
55 Quai des Grands-Augustins, Paris 6

PERGAMON PRESS G.m.b.H.
Kaiserstrasse 75, Frankfurt am Main

Copyright

©

1962

Pergamon Press Ltd.

Library of Congress Card Number: 62-12993

Set in Times 10 on 12pt. by Santype, Salisbury
and printed in Great Britain by Adlard & Son, Dorking, Surrey

CONTENTS

I. ORDINARY DIFFERENTIAL EQUATIONS

1. Ordinary differential equations and finite differences	L. FOX	3
2. Methods of Runge-Kutta type	D. F. MAYERS	16
3. Prediction and correction: Deferred correction	D. F. MAYERS	28
4. Stability of step-by-step methods	D. F. MAYERS	46
5. Boundary-value problems and methods	L. FOX	58
6. Eigenvalue problems	D. F. MAYERS	73
7. Application to the one-dimensional Schrödinger equation	D. F. MAYERS	87
8. Accuracy and precision of methods	L. FOX	95
9. Chebyshev approximation	L. FOX	113
10. Chebyshev solution of ordinary differential equations	L. FOX	129

II. INTEGRAL EQUATIONS

11. Fredholm equations of second kind	D. F. MAYERS	145
12. Fredholm equations of first and third kinds	D. F. MAYERS	154
13. Equations of Volterra type	D. F. MAYERS	165
14. Singular and non-linear integral equations	D. F. MAYERS	174
15. Integro-differential equations in nuclear collision problems	R. A. BUCKINGHAM	184
16. Roothaan's procedure for solving the Hartree-Fock equation	M. J. D. POWELL	197

III. INTRODUCTION TO PARTIAL DIFFERENTIAL EQUATIONS

17. General classification. Hyperbolic equations and characteristics	L. FOX	205
18. Finite-difference methods for hyperbolic equations	L. FOX	218
19. Parabolic equations in two dimensions: I	L. FOX	230
20. Parabolic equations in two dimensions: II	L. FOX	242
21. Finite-difference formulae for elliptic equations in two dimensions	L. FOX	255
22. Direct solution of elliptic finite-difference equations	J. E. WALSH	272
23. Iterative solution of elliptic finite-difference equations	L. FOX	284
24. Singularities in elliptic equations	L. FOX	301

IV. PRACTICAL PROBLEMS IN PARTIAL DIFFERENTIAL EQUATIONS

25. Elliptic equations in nuclear reactor problems	J. E. WALSH	315
26. Solution by characteristics of the equations of one-dimensional unsteady flow	A. E. GLENNIE	325
27. Finite-difference methods for one-dimensional unsteady flow	N. E. HOSKIN and B. W. PEARSON	339
28. Characteristics in three independent variables	D. S. BUTLER	366
29. Quasi-linear parabolic equations in more than two dimensions: I	A. R. CURTIS	378
30. Quasi-linear parabolic equations in more than two dimensions: II	A. R. CURTIS	388
31. The linear transport equation in one and two dimensions	L. H. UNDERHILL and L. M. RUSSELL	398
32. Monte Carlo methods for neutronics problems	J. B. PARKER	423
33. Special techniques of the Monte Carlo method	I. C. PULL	442
34. Some problems in plasma physics	I. C. PYLE	458
35. Self-consistent solutions of a non-linear problem in plasma physics	H. MOTZ	469
36. Numerical weather prediction	E. KNIGHTING	478
REFERENCES		494
INDEX		502

I. ORDINARY DIFFERENTIAL EQUATIONS

CHAPTER 1

ORDINARY DIFFERENTIAL EQUATIONS AND FINITE DIFFERENCES

Introduction

1. There is no single numerical method which is applicable to *every* differential equation, or even to every *ordinary* differential equation, or which is "best possible" for every member of even the much smaller class of ordinary *linear* equations. The field is very large, and for the most economic use of our computing machine, coupled with the necessity for producing accurate answers, we need a variety of methods, each appropriate to its particular and rather small class of problems. This needs emphasis, for example because many computing machines have a single "built-in" routine for ordinary differential equations, of which the most popular is a Runge-Kutta technique, and there is a tendency, certainly among the less experienced, to use this routine on problems for which better methods are available. Here we shall discuss a variety of methods, for ordinary and partial differential equations and integral equations, pointing out their respective merits and demerits from the points of view of speed, convenience and accuracy.

By "accuracy" we mean the difference between the true solution of the problem and our computed approximation, and our aim is to limit the discrepancy to the amount justified in the particular context, and to know that this has been achieved. "Speed" and "convenience" are more difficult to define. They include both the human programming time and the machine computing time, and the latter will depend among other things on the size of its store, and even of its high-speed store relative to the less accessible "backing store". Criteria of this kind will therefore vary from one individual to another, and from one machine to another, but our comments should assist in the making of any particular decision.

2. The large variety of possible problems makes it difficult to produce a useful classification. For ordinary differential equations the linear case has simplifications lacking in the non-linear case, notably in the possibility of "superposition" of partial solutions, for example as a linear combination of particular integrals and complementary solutions. But other factors may have greater importance, for example the "associated conditions", which are

generally equal in number to the order of the differential equation, and which are necessary to provide a unique solution. If these are specified at a single value of the independent variable we have an "initial-value" problem, whereas if they are shared among two or more points in a given range we have a "boundary-value" problem. A combination of differential equations and associated conditions will be called a differential system, and a non-linear initial-value system may in certain cases involve less computation and fewer storage problems than a linear boundary-value system.

The actual form of the equation is another important consideration. For example a non-linear initial system with an equation like

$$y'' = f(x, y), \quad (1)$$

which is linear in its second derivative and which lacks a first derivative, is more easily and accurately solved, by finite-difference methods, than the non-linear

$$yy'' + \sin y' = f(x, y), \quad (2)$$

for which reduction to simultaneous first-order equations and the use of Runge-Kutta methods is probably preferable.

Finally the form of the solution, and in particular its asymptotic behaviour in an infinite range of the independent variable, will often dictate the choice of method. Here we are concerned with the problem of stability, to ensure that our method produces no "spurious solutions" which, introduced perhaps through our inability to work with an infinite number of figures, may grow without bound and "swamp" the true solution.

Such considerations for ordinary differential equations apply also to the numerical treatment of partial differential equations and integral equations, and other special points will be introduced in the appropriate context.

Finite differences

3. Most methods of solution assume that the wanted function can be represented in a specified range, and to a sufficient degree of accuracy, either by a single polynomial, which might be a truncated Chebyshev series, or by a set of smoothly interlacing polynomials, which might be the truncated Taylor's series with origins at the successive pivotal points of the range, or the polynomial which passes through a certain number of selected pivotal points.

All finite-difference formulae are based on polynomial approximation, and give exact results if the function concerned is a polynomial. In other cases the formulae are approximations, and are usually written in the form of infinite series of differences. It is necessary either that the series should converge, or that the error caused by truncation after a certain number of

terms should be suitably small. Before discussing this we give some formulae which will be needed in applications.

4. We use the now standard notations

$$\left. \begin{aligned} \Delta y_r &= y_{r+1} - y_r, & \nabla y_r &= y_r - y_{r-1} \\ \delta y_r &= y_{r+\frac{1}{2}} - y_{r-\frac{1}{2}}, & \mu y_r &= \frac{1}{2}(y_{r+\frac{1}{2}} + y_{r-\frac{1}{2}}) \end{aligned} \right\}, \quad (3)$$

where Δ , ∇ , δ and μ are the operations of forward differencing, backward differencing, central differencing and averaging. Also we have

$$E y_r = y_{r+1}, \quad h = x_{r+1} - x_r, \quad y_r = y(x_r), \quad (4)$$

where E is the operation of displacement through interval h , the distance between successive pivotal points x_{r+1} and x_r , here assumed to be constant. The averaging operator is needed because the values $y_{r+\frac{1}{2}}$ and $y_{r-\frac{1}{2}}$ do not appear in the table of values, and the odd central differences $\delta^{2s+1}y_r$ are similarly lacking. On the other hand

$$\mu \delta y_r = \delta(\mu y_r) = \frac{1}{2}(\delta y_{r+\frac{1}{2}} + \delta y_{r-\frac{1}{2}}) = \frac{1}{2}(\Delta y_r + \nabla y_r), \quad (5)$$

of which both terms are present in the difference table.

For most purposes the operators can be manipulated with ordinary algebraic rules, and used formally to produce finite-difference expressions for various purposes. For example we can write $E = 1 + \Delta$, and

$$\begin{aligned} E^p y_r &= y(x_r + ph) = (1 + \Delta)^p y_r = [1 + p\Delta + \binom{p}{2}\Delta^2 + \dots] y_r \\ &= y_r + p(\Delta y_r) + \binom{p}{2}\Delta^2 y_r + \dots, \end{aligned} \quad (6)$$

a series of forward differences of y_r . This gives a finite-difference formula for the calculation of $y(x_r + ph)$ in the form of an infinite series, which terminates if p is an integer, giving the corresponding pivotal value, or if $\Delta^s y_r = 0$ for all s greater than a certain integer n , in which case $y(x)$ is a polynomial of degree n .

We can also record the operational identities

$$\delta = E^{\frac{1}{2}} - E^{-\frac{1}{2}}, \quad \mu = \frac{1}{2}(E^{\frac{1}{2}} + E^{-\frac{1}{2}}), \quad \mu^2 = 1 + \frac{1}{4}\delta^2, \quad (7)$$

so that, for example,

$$1 = \mu\mu^{-1} = \mu(1 + \frac{1}{4}\delta^2)^{-\frac{1}{2}} = \mu(1 - \frac{1}{8}\delta^2 + \frac{3}{128}\delta^4 - \dots). \quad (8)$$

This provides a method of introducing the averaging operator, which is necessary in expressions involving $\mu\delta^{2s+1}y_r$ and $\mu\delta^{2s}y_{r+\frac{1}{2}}$, respectively the odd central differences at pivotal points and the even central differences at "half-way" points.

We also use the operator for differentiation, defined by

$$D^*y = d^*y/dx^*, \quad (9)$$

and note the formal equivalence of

$$\begin{aligned} Ey_r = y_{r+1} &= y_r + hy'_r + \frac{h^2}{2!} y''_r + \dots \\ &= \left(1 + hD + \frac{h^2}{2!} D^2 + \dots\right) y_r = e^{hD} y_r, \end{aligned} \quad (10)$$

so that

$$E = e^{hD}, \quad hD = \ln E. \quad (11)$$

The replacement of E by its various difference equivalents will give formulae for derivatives.

Finally, we associate the operation of indefinite integration with D^{-1} , so that for a definite integral we write

$$\int_a^b y \, dx = D^{-1}(y_b - y_a), \quad (12)$$

and suitable formulae can be obtained by expressing D^{-1} in terms of differences.

Finite-difference formulae

5. We give now the first few terms in various formulae which will be needed in applications. For interpolation we have the forward-difference formula

$$y(x_r + ph) = y_r + p\Delta y_r + \left(\frac{p}{2}\right)\Delta^2 y_r + \dots, \quad (13)$$

which is used near the end of a range where central differences are not tabulated, and the Everett central-difference formula

$$\begin{aligned} y(x_r + ph) &= qy_r + py_{r+1} + E_2(p)\delta^2 y_r + E_2(q)\delta^2 y_{r+1} + \\ &\quad + E_4(p)\delta^4 y_r + E_4(q)\delta^4 y_{r+1} + \dots, \end{aligned} \quad (14)$$

where $q = 1 - p$ and the Everett coefficients E_2 , are known polynomials in p . These coefficients, and similar quantities involved in interpolation formulae, are tabulated, for example in N.A.O. (1956).

6. For our present purpose formulae for derivatives and integrals are of more general interest. For first derivatives at pivotal points we have

$$hy'_r = (\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \dots)y_r, \quad (15)$$

which uses the forward differences at the relevant point, and

$$hy'_r = (\Delta + \frac{1}{2}\Delta^2 - \frac{1}{6}\Delta^3 + \dots)y_{r-1}, \quad (16)$$

which uses the forward differences at the previous point. This idea can be extended, but where possible we would use the central-difference formula

$$hy'_r = (\mu\delta - \frac{1}{6}\mu\delta^3 + \frac{1}{120}\mu\delta^5 - \dots)y_r. \quad (17)$$

With central differences we have also a simple and useful formula for the derivative at a half-way point, given by

$$hy'_{r+\frac{1}{2}} = (\delta - \frac{1}{24}\delta^3 + \frac{3}{640}\delta^5 - \dots)y_{r+\frac{1}{2}}. \quad (18)$$

Similarly for second derivatives we have the forward-difference formulae

$$h^2y''_r = (\Delta^2 - \Delta^3 + \frac{1}{12}\Delta^4 - \frac{5}{24}\Delta^5 + \dots)y_r, \quad (19)$$

$$h^2y''_r = (\Delta^2 - \frac{1}{12}\Delta^4 + \frac{1}{12}\Delta^5 - \dots)y_{r-1}, \quad (20)$$

and the more valuable central-difference expressions

$$h^2y''_r = (\delta^2 - \frac{1}{12}\delta^4 + \frac{1}{90}\delta^6 - \dots)y_r, \quad (21)$$

$$h^2y''_{r+\frac{1}{2}} = (\mu\delta^2 - \frac{5}{24}\mu\delta^4 + \frac{25}{3780}\mu\delta^6 - \dots)y_{r+\frac{1}{2}}. \quad (22)$$

Formulae for higher derivatives will be given when required.

7. For definite integrals, between two pivotal points, we have the "closed" formulae, which use the integrand at both end points, and the "open" formulae, which omit one or both end points, and which have important applications in the "predictor-corrector" methods for solving differential equations. For example,

$$\int_{x_r}^{x_{r+1}} y \, dx = h(1 + \frac{1}{2}\nabla + \frac{5}{12}\nabla^2 + \dots)y_r, \quad (23)$$

is a typical open formula, and the corresponding closed formula is

$$\int_{x_r}^{x_{r+1}} y \, dx = h(1 - \frac{1}{2}\nabla - \frac{1}{12}\nabla^2 - \dots)y_{r+1}. \quad (24)$$

Similar formulae exist for integration over more than one interval, for example

$$\int_{x_r}^{x_{r+2}} y \, dx = h(2 + \frac{1}{3}\nabla^2 + \frac{1}{3}\nabla^3 + \frac{29}{90}\nabla^4 + \dots)y_{r+1}, \quad (25)$$

and
$$\int_{x_r}^{x_{r+2}} y \, dx = h(2 - 2\nabla + \frac{1}{3}\nabla^2 - \frac{1}{90}\nabla^4 + \dots)y_{r+2}. \quad (26)$$

In these formulae the terms involve differences at one point only, and we have corresponding central-difference formulae such as

$$\int_{x_r}^{x_{r+1}} y \, dx = h(\mu - \frac{1}{12}\mu\delta^2 + \frac{1}{720}\mu\delta^4 - \dots)y_{r+\frac{1}{2}}, \quad (27)$$

$$\text{and} \quad \int_{x_{r-\frac{1}{2}}}^{x_{r+\frac{1}{2}}} y \, dx = h(1 + \frac{1}{24}\delta^2 - \frac{1}{720}\delta^4 + \dots)y_r, \quad (28)$$

for integration over one interval, and the useful

$$\int_{x_{r-1}}^{x_{r+1}} y \, dx = 2h(1 + \frac{1}{6}\delta^2 - \frac{1}{180}\delta^4 + \dots)y_r, \quad (29)$$

for integration over two intervals.

These formulae can be summed to cover an extended range, and thereby become "full" quadrature formulae. They can then be written as simple weighted sums of the integrand plus a correction in terms of differences at the two end points. For example we have

$$\int_{x_r}^{x_n} y \, dx = h\{(\frac{1}{2}y_r + y_{r+1} + \dots + y_{n-1} + \frac{1}{2}y_n) + (-\frac{1}{12}\nabla - \frac{1}{24}\nabla^2 - \dots)y_n + (\frac{1}{12}\Delta - \frac{1}{24}\Delta^2 + \dots)y_r\}, \quad (30)$$

the Gregory formula which uses "sloping-difference" corrections, and

$$\int_{x_r}^{x_n} y \, dx = h\{(\frac{1}{2}y_r + y_{r+1} + \dots + y_{n-1} + \frac{1}{2}y_n) + (-\frac{1}{12}\mu\delta + \frac{1}{720}\mu\delta^3 - \dots)(y_n - y_r)\}, \quad (31)$$

the corresponding central-difference formula. Similarly, for integration between half-way points, we have

$$\int_{x_{r-\frac{1}{2}}}^{x_{r+\frac{1}{2}}} y \, dx = h\{(y_r + y_{r+1} + \dots + y_{n-1} + y_n) + (\frac{1}{24}\delta - \frac{1}{720}\delta^3 + \dots)(y_{n+\frac{1}{2}} - y_{r-\frac{1}{2}})\}. \quad (32)$$

Formulae (30) and (31) represent the "trapezium rule" plus a correction. We can similarly obtain Simpson's rule with correction, used for integrating over an even number of intervals, by expressing the differences up to δ^2 in (29) in terms of pivotal values, obtaining

$$\int_{x_{r-1}}^{x_{r+1}} y = \frac{h}{3}(y_{r-1} + 4y_r + y_{r+1}) - \frac{1}{90}h\delta^4 y_r + \dots, \quad (33)$$

which may be used for integrating differential equations, and

$$\int_{x_{r-n}}^{x_{r+n}} y \, dx = \frac{h}{3} (y_{r-n} + 4y_{r-n+1} + 2y_{r-n+2} + \dots + 4y_{r+n-1} + y_{r+n}) - \frac{1}{90} h (\delta^4 y_{r-n+1} + \delta^4 y_{r-n+3} + \dots + \delta^4 y_{r+n-3} + \delta^4 y_{r+n-1}) + \dots, \quad (34)$$

which is a full quadrature formula.

8. In all these integration formulae the result is expressed as a combination of pivotal values of the integrand, together with a correction involving series of differences of the integrand. By differentiation we also obtain a relation between pivotal values and derivatives, with a correction involving differences of the derivative. For example equation (28), treated in this way, can be written as

$$y_{r+\frac{1}{2}} - y_{r-\frac{1}{2}} = \delta y_r = h(1 + \frac{1}{24}\delta^2 - \frac{1}{3760}\delta^4 + \dots)y'_r. \quad (35)$$

The inversion and introduction of μ in the form

$$h y'_r = (1 + \frac{1}{24}\delta^2 - \frac{1}{3760}\delta^4 + \dots)^{-1} \mu^{-1} (\mu \delta y_r) \quad (36)$$

will ultimately produce formula (17), and to this extent the formulae for integration and those for differentiation are effectively equivalent.

There are, however, important differences in the way we express the correcting terms. For example we can produce from (27) the form

$$y_{r+1} - y_r = \frac{1}{2} h (y'_{r+1} + y'_r) + (-\frac{1}{12}\mu\delta^2 + \frac{1}{720}\mu\delta^4 - \dots) h y'_{r+\frac{1}{2}}, \quad (37)$$

which might be used as a rather late corrector in a predictor-corrector method. Similarly (24) gives

$$y_{r+1} - y_r = \frac{1}{2} h (y'_{r+1} + y'_r) + (-\frac{1}{12}V^2 + \dots) h y'_{r+1}, \quad (38)$$

which can be used, at an earlier stage, for the same purpose. But by operating with μ in equation (18), and expressing μ on the right in terms of δ , we find

$$y_{r+1} - y_r = \frac{1}{2} h (y'_{r+1} + y'_r) + (-\frac{1}{12}\delta^3 + \frac{1}{120}\delta^5 - \dots) y_{r+\frac{1}{2}}, \quad (39)$$

and the "correction" on the right is here given in terms of the function rather than its derivative. Such a formula is more valuable for the "deferred-correction" methods of solving differential equations, in which the derivatives of the required function need never be recorded and often not even calculated.

Similar remarks connect double integrals with formulae for the second derivative. For example, (21) gives

$$h^2 y''_r = \delta^2 y_r + (-\frac{1}{12}\delta^4 + \frac{1}{90}\delta^6 - \dots) y_r, \quad (40)$$

a useful “deferred correction formula”, but we can also invert it to find

$$\delta^2 y_r = (1 + \frac{1}{12}\delta^2 - \frac{1}{240}\delta^4 + \dots)h^2 y'' \quad (41)$$

which can be used as a “corrector”, particularly for second-order differential equations in which the first derivative is absent.

Lagrangian formulae and rounding errors

9. If we are given, or have produced in some way, a table of values of a particular $y(x)$, and we wish to interpolate, differentiate, or integrate, the difference table gives valuable information, for example about possible errors in the pivotal values, the adequacy of polynomial representation at this particular interval, the number of differences that should be used in each particular formula, and the propinquity of a possible singularity in $y(x)$ or one of its derivatives.

The storage of the difference table in the computing machine, however, may be prohibited by the size of the total store, and of the problem. Moreover, automatic assessment of a given situation is by no means trivial. For this reason it is not uncommon, particularly in automatic computation, to decide in advance the orders of differences which can safely be neglected, and to express all differences retained in terms of pivotal values. Formula (21), for example, may be written as

$$h^2 y'' = y_{r+1} - 2y_r + y_{r-1} - \frac{1}{12}\delta^4 y_r + \dots, \quad (42)$$

or as

$$h^2 y'' = \frac{1}{12}(-y_{r+2} + 16y_{r+1} - 30y_r + 16y_{r-1} - y_{r-2}) + \frac{1}{90}\delta^6 y_r + \dots, \quad (43)$$

corresponding respectively to the neglect of differences higher than the second and fourth.

Such formulae are called Lagrangian formulae, and any decision about their suitable order is usually supported by *a priori* knowledge or experimental computation, or by *a posteriori* consideration of some kind, such as reduction of the interval and checks for consistency.

10. The Lagrangian formulae are also valuable in one other respect, that of assessing the possible maximum error in any finite-difference result due to possible rounding errors in the pivotal values, assuming that these errors do not affect the negligibility of higher-order terms. For example, if each pivotal value has a possible half-unit error in (43), the maximum possible error in $h^2 y''$ is half the sum of the absolute values of the coefficients (since the errors may have either sign), which is here about $8/3$ units. The same result is obtained in this case by adding together the maximum error in each difference in the corresponding formula (21), keeping only δ^2 and δ^4 . In general, however, the latter method may give an overestimate, unless we pay