The deferred approach to the limit in ordinary differential equations

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The numerical solution of second order differential equations is studied in the limit as $h \to 0$. The form of the error is derived in a number of singular cases where the simple formulation breaks down.

The application of the method known as "Richardson extrapolation" or the "deferred approach to the limit" to the numerical solution of ordinary differential equations was considered recently by Fox (1962). In this paper we shall continue the discussion of two particular problems, arising from systems which involve a derivative in a boundary condition, and systems containing some form of singularity.

For convenience we restrict the discussion to the quasi-linear second-order equation

$$p(x)y'' + q(x)y' = f(x, y), \tag{1}$$

although the same process can be applied to other types. The equation is solved numerically by the simplest finite-difference approximation

$$h^{-2}p_n\delta^2 y_n + h^{-1}q_n\mu\delta y_n = f(x_n, y_n). \tag{2}$$

We now wish to consider the behaviour of this approximate solution as $h \to 0$. Fox showed that in general the difference from the true solution is $O(h^2)$; we consider two special cases which may give rise to different behaviour. First, if one of the boundary conditions involves a derivative, we wish to know how the result depends on the method of incorporating this derivative into the finite-difference scheme. Second, we shall study the effect of various singularities on the solution.

Let $Y(x)$ be the true solution of the differential equation, and $y(x, h)$ the solution of the approximate equation (2), using interval h; the values of $y(x, h)$ will, of course, be obtained only at values of x which are integral multiples of h. For the moment we shall assume that an expansion of the form

$$Y(x) - y(x, h) = A(x)h + B(x)h^2 + C(x)h^3 + \dots \tag{3}$$

is valid; later we shall return to the question of the existence and convergence of this expansion when the equation has a singularity. Notice that we have expanded the error in the approximate solution in powers of h, the coefficients being functions of x only.

We now substitute this expression for $y(x, h)$ in the defining equation (2) and replace the difference operators by their expansions in derivatives, giving

$$p\left(D^2 + \frac{1}{12}h^2D^4 + \frac{1}{360}h^4D^6 + \dots\right)(Y - Ah - Bh^2 - Ch^3 - \dots)$$
$$+ q\left(D + \frac{1}{6}h^2D^3 + \frac{1}{120}h^4D^5 + \dots\right)(Y - Ah - Bh^2 - Ch^3 - \dots)$$
$$= f(x, Y - Ah - Bh^2 - Ch^3 - \dots). \tag{4}$$

As this relation is an identity we may equate coefficients of powers of h, the first three terms giving

$$pD^2Y + qDY = f(x, y) \tag{5}$$

$$pD^2A + qDA = A\partial f/\partial Y \tag{6}$$

$$pD^2B + qDB = B\partial f/\partial Y + \frac{1}{12}pD^4Y + \frac{1}{6}qD^3Y - \tfrac{1}{2}A^2\partial^2 f/\partial Y^2. \tag{7}$$

The first of these simply requires that $Y(x)$ is the true solution of the original equation (1). Each succeeding equation of the system then defines the next term of the expansion (3) in terms of its predecessors.

The solution of equation (6) depends on the form of the boundary conditions; here we consider two possibilities. Suppose first that both boundary conditions involve values of the function only, say

$$Y(a) = \alpha, \quad Y(b) = \beta. \tag{8}$$

These values will be used unchanged in the numerical solution of the equation (2), so that

$$y(a, h) = \alpha, \quad y(b, h) = \beta \quad \text{for all } h. \tag{9}$$

Hence $A(a) = A(b) = 0, \quad B(a) = B(b) = 0, \dots.$ (10)

Now the solution of (6) with boundary conditions $A(a) = A(b) = 0$ will be $A(x) = 0$; a non-trivial solution can arise only in a singular case which we shall not consider here. For the same reason we find that $C(x) = 0$, and so on. The expansion (3) then becomes an expansion in even powers of h only, and the extrapolation is $O(h^2)$.

Boundary condition involving a derivative

If either of the boundary conditions involves a derivative the situation is different; the form of extrapolation may depend on the approximation used to represent the derivative. Suppose, for example, that the boundary conditions (8) are replaced by the initial values

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$$Y(a) = \alpha, \quad Y'(a) = \gamma, \tag{11}$$

and these are approximated by

$$y(a, h) = \alpha, \quad h^{-1}\mu\delta y(a, h) = \gamma. \tag{12}$$

The derivative condition then gives the relation

$$\left(D + \frac{1}{6}h^2D^3 + \frac{1}{120}h^4D^5 + \ldots\right)$$
$$(Y(a) - hA(a) - h^2B(a) - \ldots) = \gamma, \tag{13}$$

from which, by equating coefficients of powers of h, we obtain

$$\left.\begin{aligned} DY(a) &= \gamma \\ DA(a) &= 0 \\ DB(a) &= \tfrac{1}{6}D^3Y(a) \end{aligned}\right\}, \tag{14}$$

and so on. The boundary conditions for $A(x)$ in equation (6) are now $A(a) = 0$, $A'(a) = 0$, and again we have the trivial solution $A(x) = 0$. It is easily verified as before that the expansion (3) still contains even powers only.

The vanishing of the odd powers of h depends on the use of central differences throughout the calculation. If instead of (12) to represent the derivative boundary condition we had used the simple forward difference

$$h^{-1}\Delta y(a) = \gamma, \tag{15}$$

the identity (13) is replaced by

$$(D + \tfrac{1}{2}hD^2 + \tfrac{1}{6}h^2D^3 + \ldots)$$
$$(Y(a) - hA(a) - h^2B(a) - \ldots) = \gamma. \tag{16}$$

We now equate coefficients of h, giving

$$DA(a) = \tfrac{1}{2}D^2Y(a), \tag{17}$$

so that $A(x)$ is now the solution of the homogeneous equation (6) with boundary conditions $A(a) = 0$, $A'(a) = \frac{1}{2}Y''(a)$. The solution of this system will not in general be zero; we therefore find that the odd powers appear in the expansion (3) and we have h-extrapolation.

A more important practical possibility is the use of the initial conditions (11) with some form of series expansion method to give the exact value of $y(a + h)$, the remaining values being obtained by recurrence from (2). The boundary conditions (12) for $y(a)$ are now replaced by

$$y(a, h) = Y(a), \quad y(a + h, h) = Y(a + h), \tag{18}$$

or

$$hA(a + h) + h^2B(a + h) + h^3C(a + h) \ldots = 0. \tag{19}$$

By equating to zero the powers of h in this expansion we obtain

$$A(a) = 0, \tag{20}$$

$$A'(a) + B(a) = 0, \tag{21}$$

$$\tfrac{1}{2}A''(a) + B'(a) + C(a) = 0, \tag{22}$$

$$\tfrac{1}{6}A'''(a) + \tfrac{1}{2}B''(a) + C'(a) + D(a) = 0, \tag{23}$$

etc., and as before

$$A(a) = B(a) = C(a) = D(a) \ldots = 0. \tag{24}$$

Clearly $A'(a) = 0$ showing that $A(x) = 0$ for all x, and we again have h^2-extrapolation. The equation for $B(x)$ is, however, not homogeneous, so that $B(x)$ is not in general zero. Hence in (23) $C'(a)$ will not be zero, and a term in h^3 will appear in the expansion (3).

If a series expansion method is used to obtain $y(a + h)$ to start off a step-by-step integration process, we have now shown that the expansion (3) will contain both odd and even powers of h. This means that, if we use the h^2-extrapolation process to eliminate the h^2 term from the expansion, the remaining error will be of order h^3, and therefore larger than if we had approximated the derivative in the boundary condition by a central difference.

This analysis is illustrated by an example taken from Fox (1962), § 21. We solve the equation $y'' = 12x^2$ with $y(0) = 0$, $y'(0) = 0$, whose solution is $Y = x^4$. Use of the central-difference formula $\mu\delta y(0) = 0$ for the second boundary condition gives the results

$h = 1$	x	0	1	2		
	y	0	0	12		,
$h = \frac{1}{2}$	x	0	$\frac{1}{2}$	1	$1\frac{1}{2}$	2
	y	0	0	0·75	4·5	15 .

h^2-extrapolation then gives the correct results $y(1) = 1$, $y(2) = 16$.

Now we use the same recurrence relation but with the exact initial conditions $y(0) = 0$, $y(h) = h^4$; we obtain

$h = 1$	x	0	1	2		
	y	0	1	14		,
$h = \frac{1}{2}$	x	0	$\frac{1}{2}$	1	$1\frac{1}{2}$	2
	y	0	$\frac{1}{16}$	$\frac{7}{8}$	$\frac{75}{16}$	$\frac{61}{4}$,

and here h^2-extrapolation gives the inaccurate results $y(1) = \dfrac{5}{6}$, $y(2) = \dfrac{47}{3}$.

In this very simple example the recurrence relation is

$$y_{n+1} - 2y_n + y_{n-1} = 12h^2x_n^2 = 12n^2h^4, \tag{25}$$

whose explicit solution is

$$y_n = h^4(n^4 - n^2) + pn + q, \tag{26}$$

that is

$$y(x, h) = x^4 - h^2x^2 + p\frac{x}{h} + q, \tag{27}$$

where p and q are arbitrary constants. Since $y(0, h) = 0$ we see that $q = 0$ in both cases. In the first solution the condition $\mu\delta y(0) = 0$ means that $p = 0$, but if we require that $y(h, h) = h^4$ we obtain $p = h^4$ and hence $y(x, h) = x^4 - h^2x^2 + h^3x$, giving rise to the term in h^3.

It may be noted that if we intend to use only a straightforward recurrence process with fixed interval h, the use of the exact starting value $y(h, h)$ gives a slightly smaller error, $h^2(x - h)x$, than use of the central-difference approximation which gives the error h^2x^2. It is only when we use the h^2-extrapolation process that the advantage of the central-difference approximation arises.

Singularities

We now consider the effect of singularities on the extrapolation process, and begin with the example discussed by Fox (1962), § 22. The function $Y = \frac{1}{2}x^2 \log x$ satisfies the system

$$xy'' - y' - x = 0, \quad y(0) = y(1) = 0. \qquad (28)$$

Numerical results strongly suggest that the normal h^2-extrapolation is not valid in this case, and the above analysis soon confirms this result. If we simply apply the process described above we find first that $A(x)$ is identically zero and that $B(x)$ satisfies

$$\begin{aligned} xB'' - B' &= \frac{1}{12}xY^{iv} - \frac{1}{6}Y''' \\ &= -\tfrac{1}{4}x^{-1} \quad \text{and} \quad B(0) = B(1) = 0. \end{aligned} \qquad (29)$$

The general solution of this differential equation is

$$B(x) = \tfrac{1}{8}\log x + px^2 + q, \qquad (30)$$

and it is obvious that no choice of the arbitrary constants p and q can satisfy the boundary condition $B(0) = 0$.

We notice that all derivatives of $Y(x)$ of second and higher order are infinite at $x = 0$, which invalidates the expansions used in equation (4). The derivatives are given by $d^rY/dx^r = (-1)^{r+1}(r-3)!/x^{r-2}$ if $r > 3$; the series expansions for $\delta^2 y$ and $\mu\delta y$ are readily seen to converge only if $x \geqslant h$ and diverge in the region $0 < x < h$.

Returning to equation (1) we no longer assume an expansion (3) in powers of h, but write simply

$$\phi(x, h) = Y(x) - y(x, h). \qquad (31)$$

Corresponding to the equations (5), (6) and (7) we now find, retaining only terms of lowest order,

$$pY'' + qY' = f(x, Y)$$

$$p\phi'' + q\phi' = \frac{1}{12}h^2pY^{iv} + \frac{1}{6}h^2qY''' + \phi\partial f/\partial Y, \qquad (32)$$

the latter equation being valid only in the range $h \leqslant x \leqslant 1$.

We have already mentioned that values of $y(x, h)$ will be obtained only at discrete points separated by intervals of length h. The same is therefore true of $\phi(x, h)$, and some further investigation is necessary to justify our differentiation of this function. It is probably sufficient to define $\phi(x, h)$ at the intermediate points as the polynomial of lowest degree which fits the discrete points calculated, but it remains to be shown that the final result would be the same if some similar but different definition were used. One boundary condition, $\phi(1) = 0$ is immediately obtained. We cannot use directly the condition $\phi(0) = 0$, but as the finite-difference equation (2) was satisfied at $x = h$ we may write

$$\begin{aligned} p(h)[y(2h) - 2y(h) + y(0)] + hq(h)[y(2h) - y(0)]/2 \\ = h^2f(h). \end{aligned} \qquad (33)$$

Inserting $y(2h) = Y(2h) - \phi(2h)$, $y(h) = Y(h) - \phi(h)$, $y(0) = Y(0)$, where the values of $Y(x)$ are known, we obtain a relation between $\phi(h)$ and $\phi(2h)$ which constitutes the second boundary condition.

In our particular example the equation is

$$x\phi'' - \phi' = \frac{1}{12}h^2\left(-\frac{3}{x}\right) = -\frac{h^2}{4x}, \qquad (34)$$

with the general solution

$$\phi(x, h) = -\frac{h^2}{8}\log x + px^2 + q. \qquad (35)$$

The boundary condition $\phi(1, h) = 0$ gives $p = -q$.

The second boundary condition gives, after some manipulation and neglect of higher order terms in h, the result $p = -\dfrac{h^2}{8}\log h$.

Hence

$$\phi(x, h) \sim -\frac{h^2}{8}[(x^2 - 1)\log h + \log x], \qquad (36)$$

so that the extrapolation is in this case of order $h^2 \log h$. As in the previous example the difference equation (2) can be solved by elementary methods, giving

$$y_n = \alpha n^2 + \tfrac{1}{4}h^2(4n^2 - 1)\Sigma_n, \qquad (37)$$

where $\alpha = -(4N^2 - 1)\Sigma_N/4N^4$, $h = 1/N$ and

$$\Sigma_n = 1 + \frac{1}{3} + \frac{1}{5} + \ldots + \frac{1}{2n-1}.$$

Use of the approximation $1 + \frac{1}{2} + \frac{1}{3} + \ldots \sim \gamma + \log n$ confirms the result (36).

Fox (1962) also mentions that the same function $\frac{1}{2}x^2 \log x$ satisfies the system

$$x^2y'' - 2y - \frac{3}{2}x^2 = 0, \quad y(0) = 0, \quad y(1) = 0,$$

and that a similar numerical solution seems to indicate the validity of h^2-extrapolation. The analysis of this case is quite straightforward and gives the leading terms

$$\phi(x, h) = \frac{h^2}{24}(1 - x^2) + \frac{h^4}{240}\left(x^2 - \frac{1}{x^2}\right) + \ldots,$$

confirming the numerical results.

We now consider an example in which the solution is a perfectly well-behaved function, $Y = \frac{1}{9}x^3$, satisfying

$$xy'' + y' = x^2, \quad y(0) = 0, \quad y(1) = \frac{1}{9}. \qquad (38)$$

Again the straightforward approach leads to difficulties, as the equation (7) becomes

$$xB'' + B' = \frac{1}{9}. \qquad (39)$$

The general solution of this is $B = \frac{1}{9}x + p\log x + q$, and no particular solution can satisfy the boundary condition $B(0) = B(1) = 0$. We use the same device as in the previous example. The error now satisfies

$$x\phi'' + \phi' = \frac{1}{9}h^2. \quad (40)$$

Use of the boundary condition $\phi(1, h) = 0$ leads to the solution

$$\phi = \frac{h^2}{9}(x - 1) + p \log x. \quad (41)$$

At the point $x = h$ we have to satisfy

$$h\left[\frac{\phi(2h) - 2\phi(h)}{h^2}\right] + \left[\frac{\phi(2h)}{2h}\right] = \frac{1}{9}h^2,$$

so that
$$\frac{3}{2}\phi(2h) - 2\phi(h) = \frac{1}{9}h^3,$$

giving
$$p = \frac{1}{9}h^2/(\log h - 3 \log 2). \quad (42)$$

Thus the leading terms of the error are of order

$$\phi(x, h) = \frac{h^2}{9}(x - 1) + \frac{1}{9}\frac{h^2}{\log h}\log x. \quad (43)$$

We are usually only interested in the leading term of the error, but in a case like this the second term is large enough to affect the accuracy obtained quite considerably. Numerical solution gives the following results for $y(\frac{1}{2})$:

Interval h	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{16}$
$y(\frac{1}{2})$	0·02083	0·01594	0·01446	0·01404

the true solution being 0·01389. h^2-extrapolation from successive pairs of these values gives the results 0·01431, 0·01397, 0·01390.

This example illustrates the fact that the form of extrapolation will usually depend on the behaviour of the general solution of the differential equation, and not only on the behaviour of the particular solution determined by the boundary conditions.

The examples that we have studied have been unusual in that we were able to give explicit solutions both for the original differential equation and for the equation (32) defining the error function $\phi(x, h)$. This is not necessary, however, for the application of the method we have described; all that we need is to study the behaviour of the solutions near the singularity of the equation. We therefore give a final example of the application of the process to a common type of equation which has no exact solution in simple terms.

Consider the system

$$y'' + \left[f(x) + \frac{a}{x} - \frac{l(l + 1)}{x^2}\right]y = 0$$

$$y(0) = 0 \quad y(1) = 1, \quad (44)$$

where l is a non-negative integer, a a positive constant, and $f(x)$ a function with a convergent series expansion in powers of x. This equation has a general solution of the form

$$Y = Ay_1(x) + By_2(x),$$

where, for small x, $y_1(x) \sim x^{l+1}$ and $y_2(x) \sim x^{-l}$.

The boundary condition $y(0) = 0$ requires $B = 0$ so that the solution $y_2(x)$ does not occur; we must investigate whether or not the behaviour of $y_2(x)$ will affect the numerical solution of the system. We write $y_1(z) = x^{l+1}z_1(x)$, where $z_1(x)$ has a convergent expansion in powers of x. The error term $\phi(x, h)$ now satisfies

$$\phi'' + \left[f(x) + \frac{a}{x} - \frac{l(l + 1)}{x^2}\right]\phi = \frac{1}{12}h^2 y_1^{iv}$$
$$= \frac{1}{12}h^2(l + 1)l(l - 1)(l - 2)x^{l-3}u(x).$$

We shall expect the normal type of h^2-extrapolation to be valid unless this equation has a solution $\phi(x)$ which is not well-behaved at $x = 0$.

If we seek a particular integral of the form

$$\phi_1(x) = x^{l-1}(a_0 + a_1 x + a_2 x^2 \ldots)$$

we obtain

$$a_0(2 - 4l) = \frac{1}{12}h^2(l + 1)l(l - 1)(l - 2)u(0)$$

and a recurrence relation for the coefficients a_n in the usual way. The general solution is therefore

$$\phi(x) = Ay_1(x) + By_2(x) + \phi_1(x).$$

Provided $\phi_1(0)$ is finite there is thus no difficulty in satisfying the boundary conditions. At $x = 0$, $\phi(0) = 0$ showing that $B = 0$, and at $x = 1$, $\phi(1) = 0$ giving $A = -\phi(1)/y_1(1)$. Now when $l \geqslant 1$, $\phi_1(0) = 0$ since $\phi_1 \sim x^{l-1}$ near $x = 0$; and when $l = 0$ we notice that $a_0 = 0$ so that the leading term $a_0 x^{-1}$ vanishes. The straightforward h^2-extrapolation process is therefore valid in each case. A numerical solution confirms these results; again we give the values of $y(\frac{1}{2})$ obtained from various intervals h:

h	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{16}$
$y(\frac{1}{2})$	0·14286	0·14999	0·15178	0·15223

h^2-extrapolation from the first two gives $y(\frac{1}{2}) = 0·15237$, and from either the second and third or third and fourth the result $y(\frac{1}{2}) = 0·15238$. We notice that the error here is much more closely approximated by Bh^2 than in the previous example, where the term $h^2/\log h$ was significant.

Reference

Fox, L. (1962). (Ed.) *Numerical Solution of Ordinary and Partial Differential Equations*, Oxford, Pergamon Press, pp. 106–111.