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h^2- and h^4-extrapolation in eigenvalue problems

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1. *Introduction.* Two recent papers have discussed eigenvalue problems relating to second-order, self-adjoint differential equations from the point of view of the deferred approach to the limit in the finite-difference treatment of the problem. In both cases the problem is made definite by considering the differential equation

$$\phi''(x)+\{\lambda\rho(x)-\sigma(x)\}\phi(x)=0, \tag{1}$$

primes denoting differentiation with respect to x, with two-point boundary conditions

$$\left.\begin{aligned} A_0\phi'(0)+B_0\phi(0)&=0\\ \text{and}\qquad A_1\phi'(1)+B_1\phi(1)&=0,\end{aligned}\right\} \tag{2}$$

given at the ends of the interval $(0, 1)$. The usual finite-difference approach is to divide the range $(0, 1)$ into N equal strips of length $h = 1/N$, giving a set of $N+1$ pivotal values ϕ_n as the analogue of a solution of (1), ϕ_n denoting the pivotal value at $x = nh$. In terms of central differences we then have

$$\phi_n''=N^2(\delta^2-\tfrac{1}{12}\delta^4+\tfrac{1}{90}\delta^6-\tfrac{1}{560}\delta^8+\ldots)\phi_n \tag{3}$$

and retaining only second differences yields a finite-difference approximation $\phi_n = U_n$ to (1), where the pivotal U-values satisfy the equations

$$U_{n-1}+U_{n+1}-(2+h^2\sigma_n-h^2\Lambda\rho_n)U_n=0 \quad (n=1,2,\ldots,N-1) \tag{4}$$

defined at all internal points, together with two equations holding at the end-points and approximately satisfying the end conditions (2). Here Λ is the corresponding approximation to the eigenvalue λ. A possible finite-difference treatment of the end conditions (2) would be to replace (1) at $x = 0$ by the central-difference formula

$$\phi_{-1}+\phi_1-2\phi_0+h^2q_0\phi_0+O(h^4)=0$$

and use the corresponding result for the first derivative of ϕ, i.e.

$$\phi_1-\phi_{-1}=2h\phi_0'+\tfrac{1}{3}h^3\phi_0'''+O(h^5),$$

where $q(x) = \lambda\rho(x)-\sigma(x)$. Eliminating the external value ϕ_{-1} between these two and making use of (1) and (2) we obtain the equation

$$\phi_1-\{1-hk_0-\tfrac{1}{2}h^2q_0-\tfrac{1}{6}h^3(q_0'-k_0q_0)\}\phi_0+O(h^4)=0, \tag{5}$$

where for convenience we write $k_0 = B_0/A_0$. Similarly at $x = 1$ we obtain

$$\phi_{N-1}-\{1+hk_N-\tfrac{1}{2}h^2q_N+\tfrac{1}{6}h^3(q_N'-k_Nq_N)\}\phi_N+O(h^4)=0, \tag{6}$$

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with $k_N = B_1/A_1$. If we neglect terms in h^3 in these two they become what are usually taken to be the first approximation to the end conditions (2) to be used in conjunction with the set (4) (with the appropriate change $\phi = U$, $\lambda = \Lambda$). This, however, results in a loss of accuracy at the end-points over the general level of accuracy of the set (4), which is $O(h^4)$, so there is some justification for retaining the terms in h^3, e.g. if a difference correction method were being used they would subsequently be added as a correction term.

The solution of (4), (5) and (6) by any standard method in general yields $N+1$ independent sets of U_n-values, together with their associated eigenvalues which may generally be taken to approximate to the first $N+1$ eigensolutions of (1). In the special case

$$\phi(0) = \phi(1) = 0 \tag{7}$$

then $U_0 = U_N = 0$. Only $N-1$ pivotal values are now involved and there are only $N-1$ eigensolutions, which are obtained wholly from the set (4).

In the general case the eigenvalues Λ are functions of h. Bolton and Scoins (1) have recently considered the special case $\rho(x) \equiv 1$ of (1), i.e. the one-dimensional Schrödinger equation, and shown that if $\sigma(x)$ is bounded in $(0, 1)$, and non-singular at the end points then

$$\Lambda(h) = \lambda + ah^2 + O(h^4). \tag{8}$$

Moreover, for the end conditions (7), $a < 0$, i.e. $\Lambda(h)$ is an underestimate of λ for small enough h. These results are an improvement on those of Bückner (2) who showed that $\Lambda(h) = \lambda + O(h^2)$, and by assuming that (8) may be extended as a series in even powers of h, Bolton and Scoins use the deferred approach to the limit to extrapolate to zero mesh size from known values of Λ for given values of N. It is known that this type of h^2-extrapolation can lead to considerably improved estimates of the eigenvalues and also (though the practical difficulties of extrapolation are greater) to improved eigenfunctions (cf. Fox (3), p. 332). More recently Osborne (4) has considered the problem of h^2-extrapolation using very similar basic principles to those of Bolton and Scoins, viz. for a given eigensolution the eigenvalue λ and each pivotal ϕ-value is expanded as a power series in h. In fact, Osborne's expansion

$$\lambda(h) = \sum_{m=0}^{\infty} \frac{h^m}{m!} \frac{d^m\lambda(0)}{dh^m}$$

can readily be identified with (8), for he finds that $d\lambda(0)/dh = 0$ and the coefficient of h^2, which he explicitly evaluates, is easily shown to be the same as that given by Bolton and Scoins; and it is a simple matter to deduce from Osborne's results that, for the special end conditions (7), $a < 0$ provided only $\rho > 0$ throughout $(0, 1)$, a rather more general result.

Osborne suggests that for a given (small enough) value of h the coefficient a may be calculated and λ corrected according to (8), a different approach from Bolton and Scoins's extrapolation process, in which a is never explicitly calculated. This, however, ignores the effect of the change in eigenvalue on the eigenfunction with a further (consequent) change in eigenvalue, i.e. eigenvalue and eigenfunction must be consistent for *some* difference equations. These difference equations, of higher order

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accuracy than (4), are obtained in this paper. Equation (8) is replaced by the equation

$$\mu(h) = \lambda + O(h^4), \tag{9}$$

where μ is an eigenvalue of the corrected difference equations. From the μ-values we may then deduce an h^4-extrapolation process which leads to further improved estimates of the true eigenvalues of (1). The approach is somewhat different from Bolton and Scoins's and Osborne's and is based on difference approximations to the integrals obtained from the variational principle.

2. *Use of the variational method.* The Rayleigh quotient corresponding to (1) is

$$\lambda = \frac{-\int_0^1 \phi\phi''\,dx + \int_0^1 \sigma\phi^2\,dx}{\int_0^1 \rho\phi^2\,dx}. \tag{10}$$

If we express each integral in terms of pivotal ϕ-values using quadrature formulae, λ will be defined as a function of the $N+1$ values $\phi_0, \phi_1, \ldots, \phi_N$ and if we apply the variational condition $\partial\lambda/\partial\phi_n = 0$ $(n = 0, 1, \ldots, N)$ to this expression we obtain the analogue of (1) in the form of a set of difference equations. In this approach the difference problem can be formulated without introducing pivotal points outside the range of integration, even for the end conditions (2).

The first integral in the numerator of (10) is

$$\begin{aligned}\int_0^1 \phi\phi''\,dx &= (\phi\phi')_0^1 - \int_0^1 \{\phi'\}^2\,dx \\ &= k_0\phi_0^2 - k_N\phi_N^2 - \int_0^1 \{\phi'\}^2\,dx.\end{aligned}$$

To express this last integral in terms of pivotal ϕ-values consider first the restricted range $x = nh$ to $x = (n+1)h$. Expanding ϕ as a Taylor series about the point $z = x + (n+\frac{1}{2})h$, i.e.

$$\phi = \phi_{n+\frac{1}{2}} + z\phi'_{n+\frac{1}{2}} + \frac{1}{2!}z^2\phi^{\mathrm{v}}_{n+\frac{1}{2}} + \ldots \tag{11}$$

we readily obtain the usual difference formula

$$\phi_{n+1} - \phi_n = h\phi'_{n+\frac{1}{2}} + \tfrac{1}{24}h^3\phi'''_{n+\frac{1}{2}} + \tfrac{1}{1920}h^5\phi^{\mathrm{v}}_{n+\frac{1}{2}} + \ldots \tag{12}$$

so if we substitute in the integral using (11) and then eliminate $\phi'_{n+\frac{1}{2}}$ using (12) we obtain the result

$$\int_{nh}^{(n+1)h} \{\phi'\}^2\,dx = N(\phi_{n+1} - \phi_n)^2 + \tfrac{1}{12}h^3\{\phi''_{n+\frac{1}{2}}\}^2 + O(h^5). \tag{13}$$

Moreover, since

$$h\{\phi''_{n+\frac{1}{2}}\}^2 = \int_{nh}^{(n+1)h} \{\phi''\}^2\,dx + O(h^3),$$

if we make this substitution and sum (13) over all subintervals of $(0, 1)$ we have finally

$$\int_0^1 \{\phi'\}^2\,dx = N\sum_{n=0}^{N-1}(\phi_{n+1} - \phi_n)^2 + \tfrac{1}{12}h^2\int_0^1 \{\phi''\}^2\,dx + O(h^4). \tag{14}$$

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Approximations to the other integrals in (10) can be obtained using the Euler–Maclaurin formula, of which the first few terms are, for any function $f(x)$ in the range $(0, 1)$,

$$\int_0^1 f\,dx = \tfrac{1}{2}h\sum_{n=0}^{N-1}(f_n+f_{n+1}) - \tfrac{1}{12}h^2(f'_N - f'_0) + O(h^4). \tag{15}$$

Putting $f = \sigma\phi^2$ then $f' = \sigma'\phi^2 + 2\sigma\phi\phi'$, so that from the end conditions (2),

$$f'_0 = (\sigma'_0 - 2k_0\sigma_0)\,\phi_0^2 = \alpha_0\phi_0^2, \quad \text{say,} \quad \text{and} \quad f'_N = (\sigma'_N - 2k_N\sigma_N)\,\phi_N^2 = \alpha_N\phi_N^2.$$

For the other integral put $f = \rho\phi^2$ and introduce the notation $\beta_0 = \rho'_0 - 2k_0\rho_0$ and $\beta_N = \rho'_N - 2k_N\rho_N$. We then find that the Rayleigh quotient (10) can be written

$$\lambda = \frac{1}{T}\left(S + \tfrac{1}{12}h^2\int_0^1 \{\phi''\}^2\,dx\right) + O(h^4), \tag{16}$$

where S and T are functions of $\phi_0, \phi_1, \ldots, \phi_N$ given by

$$S = N\sum_{n=0}^{N-1}\{(\phi_{n+1}-\phi_n)^2 + \tfrac{1}{2}h^2(\sigma_n\phi_n^2 + \sigma_{n+1}\phi_{n+1}^2)\} - (k_0 - \tfrac{1}{12}h^2\alpha_0)\,\phi_0^2 + (k_N - \tfrac{1}{12}h^2\alpha_N)\,\phi_N^2 \tag{17}$$

and

$$T = \tfrac{1}{2}h\sum_{n=0}^{N-1}(\rho_n\phi_n^2 + \rho_{n+1}\phi_{n+1}^2) + \tfrac{1}{12}h^2(\beta_0\phi_0^2 - \beta_N\phi_N^2). \tag{18}$$

The summation in (18) is $O(1)$ and is positive provided $\rho > 0$ in $(0, 1)$ so (16) is equivalent to (8) where $a < 0$ always and Λ is an eigenvalue of the difference equations obtained by applying the condition $\partial\Lambda/\partial\phi_n = 0$ $(n = 0, 1, \ldots, N)$ to the quotient $\Lambda = S/T$. For the end conditions (7), $\phi_0 = \phi_N = 0$ and if $q(x)$ is non-singular at the end-points, the terms involving ϕ_0 and ϕ_N in (17) and (18) vanish. We then arrive at the $N-1$ equations (4) determining the approximation $\phi_N = U_N$. For the conditions (2) two further equations, obtained by putting $\partial\Lambda/\partial\phi_0 = 0$ and $\partial\Lambda/\partial\phi_N = 0$, are required. They are easily found to be

$$\left.\begin{aligned} U_1 - \{1 - hk_0 - \tfrac{1}{2}h^2q_0 - \tfrac{1}{12}h^3(q'_0 - 2k_0q_0)\}\,U_0 &= 0 \\ \text{and} \qquad U_{N-1} - \{1 + hk_N - \tfrac{1}{2}h^2q_N + \tfrac{1}{12}h^3(q'_N - 2k_Nq_N)\}\,U_N &= 0. \end{aligned}\right\} \tag{19}$$

It follows that, under the conditions stated, $\Lambda(h) < \lambda$ for any end conditions of type (2), a much more general proposition than that of Bolton and Scoins. We might also note that equations (19) are not quite the same as those obtained by neglecting terms in h^4 and putting $\phi = U$ in (5) and (6), although they agree up to terms in h^3. As a matter of passing interest we might compare these approximations by considering the specific example of the equation

$$\phi''(x) + \lambda(1 - x^2)\,\phi(x) = 0$$

with end conditions $\qquad \phi'(-1) = \phi(-1), \quad \phi'(1) = -\phi(1).$

The eigenfunctions are either even or odd functions of x and there is a simple exact solution

$$\phi(x) = e^{-\frac{1}{2}x^2}, \quad \lambda = 1$$

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corresponding to the smallest eigenvalue consistent with the end conditions. Let Λ denote the approximation to this smallest λ when (4) are taken with (19) and let Λ' correspond when (4) are taken with (5) and (6). Then we obtain the following results (where here $h = 2/N$).

Table 1

N	2	3	4	5	6
Λ	0·917237	0·967670	0·982178	0·988679	0·992154
Λ'	0·837722	0·916995	0·956484	0·971820	0·980299

3. *Higher-order approximations.* The result (16) leads at once to improved difference equations. Using the differential equation (1) and the quadrature formula (15) we obtain

$$\int_0^1 \{\phi''\}^2 dx = \int_0^1 q^2\phi^2 dx = \tfrac{1}{2}h \sum_{n=0}^{N-1} (q_n^2\phi_n^2 + q_{n+1}^2\phi_{n+1}^2) + O(h^2)$$

and (16) can be written

$$\lambda = \frac{1}{T}\left(S + \tfrac{1}{24}h^3 \sum_{n=0}^{N-1} (q_n^2\phi_n^2 + q_{n+1}^2\phi_{n+1}^2)\right) + O(h^4),$$

i.e.
$$\lambda = \mu + O(h^4). \tag{20}$$

The difference equations corresponding to the eigenvalues μ are obtained by putting $\partial\mu/\partial\phi_n = 0$ $(n = 0, 1, \ldots, N)$ and give rise to the approximation $\phi_n = V_n$, where

$$V_{n-1} + V_{n+1} - (2 - h^2q_n + \tfrac{1}{12}h^4q_n^2)V_n = 0 \quad (n = 1, 2, \ldots, N-1) \tag{21}$$

and at the end-points

$$\left.\begin{aligned} V_1 - \{1 - hk_0 - \tfrac{1}{2}h^2q_0 - \tfrac{1}{12}h^3(q_0' - 2k_0q_0) + \tfrac{1}{24}h^4q_0^2\}V_0 = 0, \\ V_{N-1} - \{1 + hk_N - \tfrac{1}{2}h^2q_N + \tfrac{1}{12}h^3(q_N' - 2k_Nq_N) + \tfrac{1}{24}h^4q_N^2\}V_N = 0. \end{aligned}\right\} \tag{22}$$

Note that in these equations we must interpret $q = \mu\rho - \sigma$, μ being only an approximation to λ; likewise in (19), $q = \Lambda\rho - \sigma$.

For the end conditions (5) we shall have $V_0 = V_N = 0$ and the finite-difference solution is completely contained in the equations (21). If we apply (21) and (22) to our previous example we obtain the results

Table 2

N	2	3	4	5
μ	0·991881	0·999030	0·999733	0·999897

so the result for $N = 2$ already reproduces the best of the results in Table 1.

4. *The deferred approach to the limit.* If the result (8) is written in its full form as a power series in h by taking more terms in the quadrature formulae it will contain only even powers of h. Bolton and Scoins make use of this result to extrapolate to zero mesh size from known values of Λ for given values of N, following Richardson's

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deferred approach to the limit. If $\Lambda(N_1)$ and $\Lambda(N_2)$ are two such values corresponding to values N_1 and N_2 of N the linear extrapolant from these two is

$$\Lambda(N_1 N_2) = \{N_1^2 \Lambda(N_1) - N_2^2 \Lambda(N_2)\}/(N_1^2 - N_2^2)$$

and similarly the quadratic extrapolant between three values of $\Lambda(N_1)$, $\Lambda(N_2)$ and $\Lambda(N_3)$ is

$$\Lambda(N_1 N_2 N_3) = \{N_1^2 \Lambda(N_1 N_2) - N_3^2 \Lambda(N_2 N_3)\}/(N_1^2 - N_3^2).$$

Table 3

N					
i	$\Lambda(i)$				
		$\Lambda(ij)$			
j	$\Lambda(j)$		$\Lambda(ijk)$		
		$\Lambda(jk)$		$\Lambda(ijkl)$	
k	$\Lambda(k)$		$\Lambda(jkl)$		$\Lambda(ijklm)$
		$\Lambda(kl)$		$\Lambda(jklm)$	
l	$\Lambda(l)$		$\Lambda(klm)$		
		$\Lambda(lm)$			
m	$\Lambda(m)$				

In this way a Neville table can be built up as, for example, in Table 3. No *a priori* information about the convergence of a given set of extrapolants in such a table is known, but very accurate estimates can usually be obtained *a posteriori* from the distribution of figures in the table. The method can be used to estimate any eigenvalue once the required approximations have been found from the difference equations.

We can obviously extend this h^2-extrapolation to a similar h^4-extrapolation based on the result (20), which can be developed in the form

$$\mu(h) = \lambda + bh^4 + ch^6 + \ldots.$$

The linear extrapolant between $\mu(N_1)$ and $\mu(N_2)$ is now

$$\mu(N_1 N_2) = \{N_1^4 \mu(N_1) - N_2^4 \mu(N_2)\}/(N_1^4 - N_2^4)$$

and in general the extrapolant between the values $\mu(N_1)$, $\mu(N_2)$, ..., $\mu(N_r)$ is

$$\mu(N_1 N_2 \ldots N_r) = \{N_1^2 S_1 \mu(N_1 N_2 \ldots N_{r-1}) - N_r^2 S_2 \mu(N_2 N_3 \ldots N_r)\}/(N_1^2 S_1 - N_r^2 S_2),$$

where $$S_1(r) = N_1^2 + N_2^2 + \ldots + N_{r-1}^2$$

and $$S_2(r) = N_2^2 + N_3^2 + \ldots + N_r^2.$$

The extrapolated values will be superior to the Λ-extrapolants or, what is more important, comparable accuracy may be obtained by solving less difference equations. To illustrate, consider an example given by Bolton and Scoins, the bounded harmonic oscillator, a classical problem in quantum mechanics. After transformation, the Schrödinger equation takes the form

$$\phi''(x) + (\lambda - \tfrac{1}{4}\xi_0^4 x^2)\,\phi(x) = 0,$$

where ξ_0 is a known constant; the boundary conditions are $\phi(\pm 1) = 0$, so $h = 2/N$. Bolton and Scoins determine the eigenvalue corresponding to the solution with no

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internal zero (the ground state) when $\xi_0 = \sqrt{2}$ by evaluating the appropriate zero of the determinant $\Delta(\Lambda) \equiv |A - \Lambda I|$ associated with (4), a simple determinant of centro-symmetric type. Results are given to nine significant figures in each of the cases $N = 2, 3, 4, 5, 6$ and from the resulting Neville table it is deduced that $\lambda = 2{\cdot}5969 \pm 0{\cdot}0002$. To carry out the corresponding problem in h^4-extrapolation we have only to find the appropriate root of the determinant associated with the equations (21), which is of the same centro-symmetric type except that for a given N it leads to a polynomial in μ of degree twice that of the corresponding polynomial in Λ. For example, when $N = 2$ the characteristic equation for μ is

$$\mu^2 - 12\mu + 24 = 0$$

whose smallest root, to four decimals, is $\mu = 2{\cdot}5359$ (cf. $\Lambda = 2$ from (4)) while when $N = 3$ we have

$$4(\mu - \tfrac{1}{9})^2 - 108(\mu - \tfrac{1}{9}) + 243 = 0$$

giving $\mu = 2{\cdot}5884$ (cf. $\Lambda = 2{\cdot}3611$). The extrapolant $\mu(23) = 2{\cdot}601$, a very accurate result for so little labour. The complete Neville table is shown below.

Table 4

N					
2	2·53589838				
		2·60133254			
3	2·58840727		2·59655279		
		2·59717416		2·59693928	
4	2·59440026		2·59690341		2·59691887
		2·59696284		2·59692029	
5	2·59591321		2·59691755		
		2·59693108			
6	2·59644021				

Successive columns of the table converge respectively upwards and downwards and from the first two columns alone we can deduce λ correct to a maximum error of five units in the fourth decimal. Rounding off to seven significant figures, we deduce from the third and fourth columns that

$$2{\cdot}596918 \leqslant \lambda \leqslant 2{\cdot}596920.$$

These limits are confirmed by the final extrapolant $\mu(23456)$ and we may fairly safely take $\lambda = 2{\cdot}596919$ correct to seven significant figures.

Similar results are obtainable from a Neville table of the μ-values given in Table 2. We can fairly safely deduce from this table that

$$0{\cdot}999998 \leqslant \lambda \leqslant 1{\cdot}000011$$

and the final extrapolant is $\mu(2345) = 1{\cdot}000003$.

Both these illustrations relate to the smallest eigenvalue of the corresponding differential equation but the method can equally be applied to higher eigenvalues. This was tested during the computations, although one has to solve more difference

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equations to obtain reasonable accuracy, as is to be expected. The calculations were carried out very rapidly on Mercury by modifications of a library subroutine for the determination of eigenvalues (and eigenvectors) of real symmetric matrices. The Neville table is then constructed by a simple programme.

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