Uniformly valid approximation of eigenvalues of Sturm—Liouville problems in geophysics

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Summary. In many geophysical applications, such as the interpretation of free oscillation periods and surface wave data, the underlying computational problem reduces to finding the eigenvalues of specific Sturm—Liouville problems. Though a variety of computational methods are available for the approximation of such eigenvalues, it is clear from the geophysical literature that the full potential which such a choice affords is not being utilized. By comparing representative methods, it is shown that, though finite difference and finite element methods are commonly proposed and used, better results are obtained when the choice is based on the nature of the eigenvalues being approximated. The results indicate clearly the advantages associated with using methods tailored to specific needs. The general conclusions are: when accuracy is the prime consideration and only the fundamental and its first few harmonics are required, most methods can be used. However, preference would be given to Prüfer phase methods, if computational efficiency were to be maximized, and to Rayleigh—Ritz methods if accuracy were the goal. When accurate uniformly valid estimates are required for long sequences of eigenvalues, the method proposed by Paine & de Hoog should be applied. If economy is a major consideration, then finite difference methods could be used in conjunction with the simple correction strategy proposed by Paine, de Hoog & Anderssen.

A comparison is made between Gilbert & Dziewonski’s program MODE and the method proposed by Paine & de Hoog.

1 Introduction

Many of the eigenvalue problems which arise in geophysical contexts possess equivalent formulations as either Sturm—Liouville eigenvalue problems of the form

\[(pu')' + qu = \lambda ru, \quad u = u(x), \quad u' = du/dx, \quad x \in (a, b),\]  

(1.1a)
\[a_1 u(a) + a_2 u'(a) = 0,\]
\[b_1 u(b) + b_2 u'(b) = 0,\]  
\[u, pu' \in C[a, b],\]  
\text{(1.1b)}

where the coefficients \(p, q\) and \(r\) are functions of \(x\) and \(a_1, a_2, b_1\) and \(b_2\) are constants; or alternatively, the minimization of Rayleigh quotients (Lagrangian integrals) of the form

\[R [u] = N [u, u]/D [u, u],\]  
\text{(1.2a)}

where

\[N [u, v] = \int_a^b (pu'v' + quv) \, dx\]  
\text{(1.2b)}

and

\[D [u, v] = \int_a^b pv dx.\]  
\text{(1.2c)}

Since, for geophysically important situations, neither equations (1.1) nor (1.2) can be solved in a simple closed form, it is necessary to adopt some numerical scheme to obtain approximations of the desired eigenvalues. But, in order to take full advantage of the variety and sophistication of available methods, it is essential to make the choice on the basis of the nature of the eigenvalues being approximated. To illustrate the range of possibilities which can arise, we consider a number of representative examples.

### 1.1 TORSIONAL EIGENFREQUENCIES \(n \sigma_l\) OF THE EARTH

Following Benioff's (1952) evidence that free oscillations of the Earth appear to be recordable for major earthquakes, the identification of free oscillation modes with periods of up to about 1 hr from the 1960 Chilean earthquake and the subsequent determination of eigenfrequencies of a large number of additional modes had a great impact on modern seismology. Each observation of a period of free Earth oscillation yields, independent of equation of state assumptions, a constraint on the possible distributions of \(\rho, \kappa\) and \(\mu\) in the Earth's interior (cf. Bullen 1975, p. 310). The use of such data to infer information about \(\rho, \kappa\) and \(\mu, or \rho, \alpha\) and \(\beta\), is unfortunately rather complex as the underlying mathematical formalism is an inverse eigenvalue problem. In particular, if the substitution \(U = rV\) is applied to the equations of Alterman, Jarosch & Pekeris (1959) for the eigenfrequencies \(n \sigma_l\) of the torsional oscillations of an SNREI earth, the following Sturm–Liouville form is obtained for \(n \sigma_l\)

\[d \left(\frac{dV}{dr}\right) + \left[r^4 \mu \frac{dV}{dr} + (r^4 \rho n \sigma_l^2 - (l^2 + l - 2)\mu r^2)\right]V = 0, \quad a < r < b,\]  
\text{(1.3)}

with boundary conditions

\[\frac{dV}{dr} = 0, \quad r = a, \quad r = b,\]  
\text{(1.4)}

where \(a\) and \(b\) denote the radius of the core–mantle boundary and the surface of the Earth, respectively. Computationally, it is often necessary to repeatedly solve equations (1.3) and (1.4) to obtain long sequences of \(n \sigma_l\)-values for fixed \(l\) and various choices of \(\rho\) and \(\mu\).
1.2 LOVE WAVES

As pointed out by Jeffreys (1962, p. 35), surface waves are as important as P and S waves in the study of Earth structure, since they have the potential to propagate to and be observed at larger distances from the source than P and S waves. For analysis and interpretation purposes, the phase velocities of such waves are usually used since they can be defined mathematically as the eigenvalues of appropriate differential equations. In particular, the phase velocities \( \xi \) of Love waves correspond to the eigenvalues of (cf. Keilis-Borok, Neigauz & Shkadinskaya 1965)

\[
\frac{d}{dz} \left( \mu \frac{dv}{dz} \right) + (p^2 \rho - \xi^2 \mu) v = 0, \quad v = v(z),
\]

subject to the boundary conditions

\[
\frac{dv}{dz} \bigg|_{z=0} = 0, \quad v(\infty) = 0,
\]

where \( p \) denotes the frequency of the Love wave. Computationally, it is usually only necessary to compute the fundamental and its first few harmonics.

1.3 RADIAL OSCILLATIONS OF THE EARTH

The importance of free oscillation data in the study of Earth structure has been discussed in Section 1.1. There are two independent forms of oscillation: torsional oscillations associated with shear wave motion and spheroidal oscillations associated with compressional wave motion. As shown in Section 1.1, the equations defining torsional oscillations (cf. equations 1.3 and 1.4) have a Sturm–Liouville representation. The equations for spheroidal oscillations are coupled (cf. Alterman, Jarosch & Pekeris 1959) and do not have a standard Sturm–Liouville representation. However, in the case of purely radial oscillations, which correspond to spheroidal oscillations with their angular order number \( l \) equal to zero, one again obtains a second-order differential equation

\[
4 \frac{d}{dr} \frac{d}{dr} U - \frac{4}{r} \rho g_0 U + \frac{d}{dr} \left[ \lambda \left( \frac{dU}{dr} + \frac{2U}{r} \right) + 2\mu \frac{dU}{dr} \right] - \mu \left( \frac{dU}{dr} - \frac{4U}{r} \right) = 0, \quad 0 < r < b,
\]

(cf. Pekeris & Jarosch 1958) along with homogeneous boundary conditions, where \( n \omega_0 \) is the angular frequency of the radial oscillation \( nS_0 \), and \( g_0 \) is the unperturbed gravitational force. In essence, the standard transformation can be introduced to reduce equation (1.7) to Sturm–Liouville form, except that the coefficients \( \rho, \lambda \) and \( \mu \) now contain discontinuities associated with the core–mantle and inner–outer core boundaries. Consequently, the coefficients of equation (1.7) fail to satisfy the standard type of regularity assumed to apply when working with second order differential equations such as Sturm–Liouville operators. Computationally, it is again necessary to repeatedly solve equation (1.7) in conjunction with its homogeneous boundary conditions to obtain long sequences of \( n \omega_0 \)-values for various choices of \( \rho, \lambda \) and \( \mu \) (cf. Wang, Cleary & Anderssen 1979).

1.4 SEISMIC RESPONSE CALCULATIONS

In earthquake engineering, the periods of the free oscillations of the structure under examination are used to evaluate its seismic response characteristics. Usually (cf. Newmark & Rosenblueth 1971, Chapter 1), only the fundamental eigenfrequency is used in seismic response estimates. Though the underlying eigenvalue problem has a Sturm–Liouville form, this fact is exploited by working directly with the corresponding variational formulation.
(cf. equation 1.2a–c), or an algebraic approximation derived from first principles (following the engineering approach to finite elements).

All methods which can be applied to either equations (1.1) or (1.2) involve two basic steps: (i) replace the exact problem with an approximate problem which is (theoretically) soluble; (ii) solve the approximate problem numerically. Clearly, the total error will be the sum of the errors associated with these two steps. Although the importance of the error introduced in the second step should not be underestimated, the most important component is that arising from the first, since the error thereby generated usually dominates all other considerations. It is the choice of the approximate problem in step (i) which should reflect most the nature of the eigenvalues to be approximated.

The aim of the present paper is to indicate how this choice should be made for the different types of Sturm–Liouville eigenvalue problems which arise in geophysical contexts. Initially, in Section 2, we discuss in some detail the crucial nature of the first step. Error estimates for a number of representative methods are given in Section 3. Taking accuracy to be the prime consideration, they are used in Section 4 to draw general conclusions about the tailoring of one's choice to the types of eigenvalues required. These conclusions are verified numerically.

When comparing methods, it is assumed that accuracy, rather than economy, should be the prime consideration. For geophysical problems, there is no point in computing eigenvalues economically, if the resulting accuracy is such that incorrect inferences are made.

When economy is a major consideration, finite difference methods could be used in conjunction with the simple correction strategy proposed by Paine, de Hoog & Anderssen (1980). This is discussed in Section 5.

Because Gilbert & Dziewonki's program MODE has been used to compute eigenfrequencies and periods for numerous Earth models, it is important to confirm that inferences based on its use are not invalid because of any numerical shortcomings in the algorithms used in MODE. This is done in Section 6.

In this paper, we restrict attention to one-dimensional Sturm–Liouville problems defined by a single two-point boundary value operator (namely, equation 1.1a–c). An examination of more complex situations, where coupling, higher dimensionality and systems of equations occur, is beyond the scope of the present discussion. However, the basic point being made here (namely, 'the choice of method should be based on the nature of the eigenvalues being approximated, if reasonable accuracy and economy are to be guaranteed') carries over.

2 Replacement of an exact eigenvalue problem by an approximate one

For mathematical reasons, which are consistent with geophysical considerations, we restrict attention to situations where the coefficients \( p, q \) and \( r \) and the boundary conditions (1.1b) are such that the spectrum \( \{\lambda\} \) of equation (1.1a–c) is positive definite, discrete and simple; namely,

\[
\{\lambda\} = \{\lambda_1, 0 < \lambda_1 < \lambda_2 < \ldots < \lambda_n < \ldots\}. \tag{2.1}
\]

Sufficient conditions which guarantee that \( \{\lambda\} \) has such properties are (see, for example, Mikhlin 1971, Chapter 6, Section 7)

(i) \( p(x), p'(x), q(x) \) and \( r(x) \) continuous on \([a, b]\),

(ii) \( p(x) \geq p_0 = \text{const.} > 0, \ q(x) \geq 0, \ r(x) \geq r_0 = \text{const.} > 0, \)

(iii) \( a_2 = b_2 = 0. \)

Not all geophysical situations are covered by these conditions. For those that are not, either a trivial change in the problem will give the desired conditions, or the more general
conditions found in Mikhlin (1971, Chapter IV, Section 24) and Achiezer & Glazman (1962) will be needed to guarantee appropriate regularity.

As mentioned in the Introduction, the strategy for finding the eigenvalues of (1.1a–c) consists of two basic steps: (i) the construction of some computational formalism which in some sense approximates the given differential eigenvalue problem; and (ii) the numerical solution of the resulting computational formalism. Examples of its application to geophysical problems can be found in Smith & Bolt (1976), Wiggins (1976) and Moon & Wiggins (1977), as well as in the references cited by Wiggins (1976).

Thus, in order to ensure that the approximate eigenvalues yield good approximations to the exact, it is not only necessary to prove that the numerical method used in (ii) yields accurate numerical estimates, but also necessary to establish that the (exact) eigenvalues of the computational formalism itself yield accurate estimates of the required differential eigenvalues.

The choice of method for carrying out step (ii) is of course important because one must necessarily have confidence in the accuracy with which the numerical estimates approximate the exact eigenvalues of the formalism chosen in step (i). But, it is readily seen that, no matter how good the methods of step (ii) are, the accuracy of the numerical estimates obtained is limited by the accuracy of the exact eigenvalues of the formalism chosen. Therefore it is this limitation which is the most important and which should be the dominant consideration in the evaluation of the effectiveness of a given method.

To illustrate the importance of this point, consider the use of a Rayleigh–Ritz procedure for approximating the eigenvalues of equation (1.1a–c).

For this procedure, step (i) amounts to replacing the given problem by an algebraic eigenvalue problem determined by the choice of some basis functions \{\phi_i^{(n)}\}_{i=1}^n; while step (ii) reduces to the (numerical) evaluation of the elements of the matrices which define the algebraic problem and the numerical solution of the algebraic problem to yield the approximate eigenvalues \{\lambda^{(n)}\} = \{\lambda_j^{(n)}\}_{j=1}^n.

The success of the Rayleigh–Ritz procedure depends heavily on the choice of basis functions \{\phi_i^{(n)}\}_{i=1}^n. For example, Mikhlin (1976, Chapter VII, Section 1) has shown that, if the basis functions are chosen to be globally defined polynomials of degree \((i + 1)\) (so that the dependence of the \(\phi_i^{(n)}(x)\) on \(n\) disappears), then there is no guarantee that the largest approximate Rayleigh–Ritz eigenvalue \(\lambda_n^{(n)}\) does not grow as rapidly as \(n^4\) whereas the growth of \(\lambda_n\) is only \(n^2\).

Though the choice of a finite element basis (for which the dependence of the \(\phi_i^{(n)}(x)\) on \(n\) is explicit) for the \{\phi_i^{(n)}(x)\}_{i=1}^n can ensure that the corresponding \(\lambda_n^{(n)}\) has the correct growth of \(n^2\), the approximate eigenvalues generated do not necessarily approximate the first \(n\) eigenvalues of \{\lambda\} to better than relative error accuracy; namely, it may only be possible to guarantee that

\[
\frac{|\lambda_j - \lambda_j^{(n)}|}{\lambda_j} \leq Cn^{-p}, \quad j = 1, \ldots, n, \quad p > 0, \tag{2.3}
\]

where \(C\) is a constant.

For example, consider the application of the Rayleigh–Ritz procedure to

\[
-u'' = \mu u, \quad u(0) = u(1) = 0, \quad x \in [0, 1], \quad u' = du/dx, \tag{2.4}
\]

when the basis functions \{\phi_i^{(n)}\}_{i=1}^n are chosen to be the linear hat functions \{l_i^{(n)}(x)\}_{i=1}^n on the uniform grid \(G\)

\[
G = \{x_i, \quad i = 0, 1, \ldots, n + 1; \quad x_{i+1} - x_i = h = 1/(n + 1), \quad i = 0, \ldots, n\};
\]
Figure 1. The linear hat functions $l_{j}^{(n)}$, $j = 1, 2, \ldots, n$ of equation (2.5).

namely (see Fig. 1),

$$l_{j}^{(n)}(x) = \begin{cases} 
\frac{(x - x_{j-1})}{h} & x_{j-1} \leq x < x_{j} \\
\frac{(x_{j+1} - x)}{h} & x_{j} \leq x < x_{j+1}
\end{cases} \quad (2.5)$$

Then, setting

$$u = \sum_{j=1}^{n} a_{j}^{(n)} \phi_{j}^{(n)}(x)$$

in equation (1.2a), the Rayleigh–Ritz equations (corresponding to $Ac - \sigma^2 Bc = 0$ on p. 137 of Wiggins 1976) become

$$A \alpha = \mu^{(n)} B \alpha$$

where $\alpha = (a_{1}^{(n)}, \ldots, a_{n}^{(n)})^{T}$ is a non-zero vector of order $n$, and $A$ and $B$ are the $n$th-order tridiagonal matrices

$$A = h^{-1} \begin{bmatrix}
2 & -1 & 0 & \cdots & 0 \\
-1 & 2 & -1 & \cdots & 0 \\
0 & \ddots & \ddots & \ddots & 0 \\
0 & \cdots & 0 & 2 & -1 \\
0 & \cdots & 0 & -1 & 2
\end{bmatrix}, \quad B = h/6 \begin{bmatrix}
4 & 1 & 0 & \cdots & 0 \\
1 & 4 & 1 & \cdots & 0 \\
0 & \ddots & \ddots & \ddots & 0 \\
0 & \cdots & 0 & 4 & 1 \\
0 & \cdots & 0 & 1 & 4
\end{bmatrix}.$$

It is not difficult to show that

$$\mu_{j}^{(n)} = 6 h^{-2} (1 - \cos j \pi h) (2 + \cos j \pi h)^{-1}. \quad (2.6)$$

Although $\mu_{j}^{(n)}$ has the correct growth of $n^2$, the sharpest possible bound of the form (2.3) which will hold for the $\{\mu^{(n)}\}$ is

$$\frac{\mu_{j} - \mu_{j}^{(n)}}{\mu_{j}} \leq C, \quad j = 1, 2, \ldots, n. \quad (2.7)$$

As Table 1 shows, such a relative error estimate is insufficient to guarantee, at least for large $j$, that $\mu_{j}^{(n)}$ yields a realistic approximation to $\mu_{j}$.

Although convergence estimates of the form (2.3) are instructive, because they give an overall picture of what can be expected of the approximations, it is not optimal because the true nature of the convergence is obliterated by the worst-case behaviour which is the basis
Approximation of eigenvalues in geophysics

Table 1. Comparison of differential eigenvalues of (2.4) with their exact Rayleigh–Ritz approximates defined by (2.6).

<table>
<thead>
<tr>
<th>i</th>
<th>$\mu_j$</th>
<th>$\mu_j^{(5)}$</th>
<th>$\mu_j^{(10)}$</th>
<th>$\mu_j^{(15)}$</th>
<th>$\mu_j^{(100)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>9.87</td>
<td>10.20</td>
<td>9.95</td>
<td>9.91</td>
<td>9.87</td>
</tr>
<tr>
<td>2</td>
<td>39.48</td>
<td>44.89</td>
<td>40.79</td>
<td>40.06</td>
<td>39.49</td>
</tr>
<tr>
<td>3</td>
<td>88.83</td>
<td>116.12</td>
<td>95.58</td>
<td>91.79</td>
<td>88.89</td>
</tr>
<tr>
<td>4</td>
<td>157.91</td>
<td>227.84</td>
<td>179.55</td>
<td>167.35</td>
<td>158.12</td>
</tr>
<tr>
<td>5</td>
<td>246.74</td>
<td>300.00</td>
<td>300.00</td>
<td>270.00</td>
<td>247.25</td>
</tr>
<tr>
<td>6</td>
<td>355.31</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>483.61</td>
<td>446.47</td>
<td>403.99</td>
<td>356.36</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>631.65</td>
<td>674.59</td>
<td>786.67</td>
<td>634.99</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>799.44</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>986.96</td>
<td>1116.01</td>
<td>1045.06</td>
<td>995.10</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>1194.22</td>
<td>1200.00</td>
<td>1350.00</td>
<td>1206.15</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>1421.22</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>1667.96</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>1934.44</td>
<td></td>
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<td></td>
</tr>
<tr>
<td>15</td>
<td>2220.66</td>
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</tr>
<tr>
<td>16</td>
<td>2526.66</td>
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<tr>
<td>17</td>
<td>2852.32</td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

of equation (2.3). This can be overcome by using order of convergence bounds which, for the above example, become

$$|\mu_j - \mu_j^{(n)}| \leq C(j)h^2 \quad n > N(j).$$

For fixed $j$, it clearly indicates the potential effectiveness of a method. However, such bounds obliterate the worst-case behaviour of equation (2.7).

Since, on their own, neither yield a clear indication of what can be expected, neither will be adequate for the evaluation and comparison of different methods for computing eigenvalues. What is required is a bound which will combine the ‘worst-case’ information contained in equation (2.3) with the ‘best-case’ information in equation (2.8). One possible form which will combine these two requirements, and which we shall adopt as the standard in this paper is

$$|\lambda_j - \lambda_j^{(n)}| \leq Ch^P\lambda_j^q$$
Table 2. Error in Moon & Wiggins (1977) estimates of the frequencies $n\sigma_l$ of torsional free oscillations $nT_l$ relative to those of Alterman et al. (1959). $n\sigma_l(A)$ denotes the frequencies obtained using the method of Alterman et al. (1959), $n\sigma_l('m')$ the frequencies obtained by Moon & Wiggins (1977) with an approximation of 'm' layers.

| Toroidal mode $nT_l$ | $n\sigma_l(A)$ | $|n\sigma_l(A) - n\sigma_l(2)|$ | $|n\sigma_l(A) - n\sigma_l(10)|$
<table>
<thead>
<tr>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>$l$</td>
<td>$n$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>5.8075</td>
<td>0.0004</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>66.6625</td>
<td>0.0146</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>209.6486</td>
<td>0.2750</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>448.3534</td>
<td>23.9855</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>782.6623</td>
<td>689.2358</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>1212.5294</td>
<td>931.2471</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>25.3504</td>
<td>0.0018</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>96.2688</td>
<td>0.0237</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>237.0064</td>
<td>0.2211</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>474.8070</td>
<td>23.6865</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>808.7754</td>
<td>702.8608</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>1238.4827</td>
<td>929.4475</td>
</tr>
</tbody>
</table>

where $C$ is a constant which is independent of $n$ and $j$. For the above example, equation (2.9) becomes

$$|\mu_j - \mu_j^{(n)}| \leq C h^2 \mu_j^2 \quad j = 1, 2, \ldots, n,$$

which compactly combines the information contained in equations (2.7) and (2.8).

To illustrate that the difficulties alluded to above do occur in the published geophysical literature, we examine the results obtained by Moon & Wiggins (1977) on the computation of the eigenfrequencies of a simple Earth model using a Rayleigh–Ritz method with Hermite cubic basis functions. For the first six eigenvalues with overtone number 2 and 4 (listed in Table 2), a comparison of the Moon & Wiggins' values with those obtained from the method proposed by Alterman et al. (1959) (which are assumed to be exact) shows clearly the high order convergence which results from increasing $n$ from 2 to 10 and the predicted rapid deterioration in the accuracy of $\lambda_k^{(n)}$ as $k$ is increased with $n$ fixed. This confirms that poor and even inferior approximations can result from the use of methods which cannot guarantee uniformly valid estimates for the eigenfrequencies, and that the Rayleigh–Ritz is not the preferred method for the calculation of free oscillation eigenfrequencies of Earth models.

In practice, the above difficulties associated with the use of the Rayleigh–Ritz method are suppressed by taking the order of the matrix eigenvalue problem to be at least an order of magnitude larger than the highest harmonic which must be estimated approximately. Though such a strategy can be used to give accurate estimates, it follows from the error estimates of Section 3 that more economical procedures exist, when long sequences of eigenvalues are required.

### 3 Error estimates for representative methods

When accuracy is taken to be the prime consideration, it is clear from the discussion of Section 2, that an effective comparison of methods must be based on the form the error estimates take for each method in a representative sample. For the representative sample...
Examined below, we give a brief description of each method along with the corresponding error estimates.

**Finite Difference Methods**

At each internal grid point $x_i (i = 1, 2, \ldots, n)$ on the following grid $G$,

$$G = \{x_i; x_i = (i - 1)h, \quad i = 0, 1, 2, \ldots, n + 1, \quad h = (b - a)/(n + 1); \}$$

the differential equation (1.1a) is replaced by a standard finite difference approximation. Taken together, this set of difference equations, in conjunction with difference approximations for the boundary conditions (1.1b), yields an algebraic eigenvalue problem of the form

$$Au = \lambda^{(n)} Bu,$$

where $A$ is an $n \times n$ matrix and $u$ is an $n$-dimensional vector.

Keller (1968) has shown that, for sufficiently small $h$, the error arising in the $\{\lambda^{(n)}\}$ is directly proportional to the truncation error associated with the particular finite difference approximation used. For example, if central differences are used, then

$$|\lambda_k - \lambda_k^{(n)}| \leq Ch^2 \lambda_k^2, \quad h < h_0(k),$$

where, here and below, $C$ denotes a constant which is bounded independently of $k$ and $h$.

**Shooting Methods**

The strategy behind this class of methods is the transformation of equation (1.1) into some equivalent boundary value problem, and then the solution of the initial value problem (IVP) which is obtained when one of the boundary conditions is replaced by an appropriate initial condition. The eigenvalues then correspond to the values of $\lambda$ for which the solution of this IVP satisfies the remaining boundary condition. In practice, they are found as the zeros of the function $\omega(\lambda)$ obtained by substituting the solution of the IVP, for a given value of $\lambda$, into the free boundary condition.

Although there are many possible ways of replacing equation (1.1) by such an IVP, we limit attention to the first-order system (see Alterman \textit{et al.} 1959).

$$u' = v/p,$$

$$v' = (q - \lambda r)u,$$

obtained from equation (1.1a) by introducing the additional variable $v = pu'$. An IVP is then obtained by using this same substitution to generate the initial conditions

$$u(a) = a_2,$$

$$v(a) = -a_1 p(a),$$

from equation (1.1b). If, for a given value of $\lambda$, the solution of this initial value problem is denoted by

$$u = [u(x, \lambda), \ v(x, \lambda)]^T,$$

then the eigenvalues of equation (1.1a−c) are precisely the values of $\lambda$ for which $u$ satisfies the boundary condition at $b$; i.e. the eigenvalues correspond to the zeros of

$$\omega(\lambda) = b_1 p(b)u(b, \lambda) + b_2 v(b, \lambda).$$
Since in general equation (3.3) cannot be integrated exactly, it is usual to use some initial value routine to obtain approximations for \( u(b, \lambda) \) and \( v(b, \lambda) \). For such methods, Keller (1968; Theorem 5.2.3) has shown (under the assumption that rounding errors and the error associated with the determination of the zeros of equation (3.5) can be ignored) that the expected accuracy of the resulting eigenvalues will have the same order of convergence as that of the method used in the integration. Thus, if the classical fourth order Runge–Kutta method is used on a uniform partition,

\[
|\lambda_k - \lambda_k^{(n)}| \leq C(k)h^4, \quad h = 1/n, \quad k < k_0(h),
\]

where \( C(k) \) depends on the error in \( u(b, \lambda) \) and \( v(b, \lambda) \), and the behaviour of \( \omega(\lambda) \) near its zeros (cf. Keller 1968; Bailey, Gordon & Shampine 1978). For example, when the local truncation error is estimated from the expansion (2–36) given in Henrici (1962), this last error estimate becomes

\[
|\lambda_k - \lambda_k^{(n)}| \leq Ch^4\lambda_k^3, \quad k < k_0(h). \tag{3.6}
\]

In reality, it is difficult to quantify the behaviour of shooting methods, since any reasonable implementation would utilize the now-readily-available variable step and variable order packages such as ‘DGEAR’ in IMSL. However, once the eigenfunction associated with the eigenvalue being estimated becomes highly oscillatory, such packages will perform the integration using very small step-lengths. While they will ultimately yield an accurate estimate, more economic methods could have been used.

Almost any root-finding procedure can be used to locate the zeros of equation (3.5). However, because of its efficiency, the method proposed by Verreault (1965) (or its modification implemented by Backus & Gilbert 1967) has major advantages over standard procedures such as Newton’s method.

Verreault observed that the stationary nature of the Rayleigh quotient at an eigenvalue can be used, together with the integration of equation (3.3) using a sufficiently accurate initial approximation of the eigenvalue, to yield a correction to the original approximation which is second-order accurate. The major advantage of this approach is that the mentioned accuracy is attained without excessive integrations of equation (3.3) and without the computationally expensive evaluation of \( \delta \omega / \delta \lambda \).

Such a strategy guarantees uniformly valid approximations, when the step length of the integration is chosen to ensure that a suitably accurate approximation to the corresponding eigenfunction is generated. Its disadvantage is the inefficiency associated with computing each approximation as a calculation independent of all others.

**Prufer Phase Methods**

Although these methods can be classified as shooting methods, they are considered separately because they behave differently from and are better than that predicted for standard shooting methods. There are a number of variants of the Prufer phase method (namely, standard, scaled and modified), but all are obtained by applying the Prufer phase transformation

\[
\tan \theta = \rho \frac{u}{pu}, \quad \theta = \theta(x, \lambda), \tag{3.7}
\]

to equation (1.1a, b), where \( \rho = \rho(x, \lambda) \) is some appropriately chosen scaling function which defines the different variants (namely, \( \rho(x, \lambda) = 1, \lambda^{1/2} \) and \( (\lambda pr - pq)^{1/2} \), respectively). All
Approximation of eigenvalues in geophysics

are based on projecting the eigenfunctions into an amplitude–phase space, in which the phase satisfies a first-order differential equation which is independent of amplitude. In fact, using the transformations (3.7), (1.1a, b) is replaced by non-linear boundary value problems of the form

\[ \theta' = f(x, \theta, \lambda), \]  
\[ \theta(a) = \alpha(\lambda), \]  
\[ \theta(b) = \beta(\lambda), \]  
where the form of \( f(x, \theta, \lambda), \alpha(\lambda) \) and \( \beta(\lambda) \) depend on the choice of \( \rho(x, \lambda) \) (cf. Paine 1979, Chapter 2). The eigenvalues are found by applying shooting methods to equations (3.8)–(3.10).

These variants perform better than standard shooting methods because the transformations (3.7) are always chosen to guarantee that the dominant behaviour of the phase \( \theta \), defined by equations (3.8)–(3.10), is linear. Thus, the numerical integration of the resulting initial value problems can be performed with greater accuracy and economy than is possible for standard shooting methods. However, rigorous proofs that quantify how Prüfer phase methods perform are complex and cumbersome (cf. Paine 1979, Chapter 2).

In a detailed analysis of Prüfer phase methods, Paine (1979) has shown that, when Huen’s method (cf. Henrici 1962, p. 67) is used to perform the integration:

- **Standard Prüfer phase method**
  \[ |\lambda_k - \lambda_k^{(n)}| < C h^2 \lambda_k (\lambda_k^{(n)})^{3/2} E(b - a), \quad \lambda_k^{(n)} h < \text{const.}, \]  

- **Scaled Prüfer phase method**
  \[ |\lambda_k - \lambda_k^{(n)}| < C h^2 \lambda_k^{1/2} (\lambda_k^{(n)})^{3/2} E(b - a), \quad \lambda_k^{(n)} h < \text{const.}, \]  

- **Modified Prüfer phase method**
  \[ |\lambda_k - \lambda_k^{(n)}| < C h^2 \lambda_k^{1/2} \lambda_k^{(n)}, \quad \lambda_k^{(n)} h < \text{const.}, \]  

where \( E(x) = [\exp (Lx) - 1]/L \) with \( L = L(\lambda) \); and, when the classical Runge–Kutta method is used to perform the integration:

- **Scaled and modified Prüfer phase methods**
  \[ |\lambda_k - \lambda_k^{(n)}| < C h^4 \lambda_k^{1/2} (\lambda_k^{(n)})^{1/2}, \]  

for suitably small \( h \) and \( 4 \lambda_k^{(n)} h^2 < \pi^2 \).

**RAYLEIGH–RITZ METHODS**

As is well known (see, e.g. Schultz 1973, Theorem 3.1), the eigenvalues \( \{\lambda_k\} \) of equation (1.1a–c) can be characterized using \( R[u] \) and \( D[u, v] \) of equations (1.2a) and (1.2c) by

\[
\lambda_k = \begin{cases} 
\inf \{ R[u]; \ u \in \mathcal{H}_0 \text{ such that } D[u, u_j] = 0, \ 1 \leq j < k \}, \\
\min_{a} \left\{ \max_{i=1}^{k} a R \left[ \sum_{i=1}^{k} a_i v_i \right]; \ v_1(x), \ldots, v_k(x) \in \mathcal{H}_0 \text{ are linearly independent} \right\}, 
\end{cases}
\]  
(3.15)
where $\mathcal{H}_0$ denotes the functions with piecewise continuous first derivatives which are square summable and satisfy the boundary conditions (1.1b) and (1.1c), $\{u_k\}_{k=1}^\infty$ denotes the eigenfunctions corresponding to the eigenvalues $\{\lambda_k\}$, and $a = (a_1, a_2, \ldots, a_n)^T$. Let $\mathcal{F}_n$ denote an $n$-dimensional subspace of $\mathcal{H}_0$ with span $\{\phi_i(x)\}_{i=1}^n$. The Rayleigh–Ritz method consists of looking for the minima of $R[u]$ on $\mathcal{F}_n$. The restriction of $R[u]$ to $\mathcal{F}_n$ yields the following algebraic eigenvalue problem

$$Aa = \lambda Ba, \quad a = (a_1, a_2, \ldots, a_n)^T,$$

where $A$ and $B$ denote $(n \times n)$ matrices with entries

$$A_{ij} = D(\phi_i, \phi_j), \quad B_{ij} = N(\phi_i, \phi_j).$$

Since $A$ and $B$ are symmetric and positive definite, the matrix eigenvalue problem yields the approximations $0 < \lambda_1^{(n)} < \lambda_2^{(n)} < \ldots < \lambda_n^{(n)}$.

The actual implementation of the method depends heavily on the choice of the basis $\{\phi_i\}_{i=1}^n$. On the one hand, if the $\{\phi_i\}_{i=1}^n$ correspond to arbitrarily chosen globally defined coordinate functions then the rate of growth of $\lambda_n^{(n)}$ can often exceed that of $\lambda_n$. On the other, if the $\{\phi_i\}_{i=1}^n$ correspond to the eigenfunctions of an operator similar to equation (1.1a–c), then the rate of growth of $\lambda_n^{(n)}$ matches that of $\lambda_n$. A fuller discussion can be found in Mikhlin (1976, Chapter VII).

Often, the $\{\phi_i\}_{i=1}^n$ are chosen to be piecewise polynomials on a uniform partitioning of $[a, b]$ (cf. Mikhlin 1976, Chapter VII; Schultz 1973, Chapter I). When the polynomials are linear, the error is essentially the same as that for finite difference methods (cf. Schultz 1973, p. 120; and Section 2 in this paper). If a cubic Hermite basis is used, Birkhoff et al. (1966) have shown that

$$|\lambda_k - \lambda_k^{(n)}| \leq C \sum_{j=1}^k |\lambda_k^j| h^6, \quad h < h_0(k).$$

### The Similar Operator Implementation for the Rayleigh–Ritz Method

The deterioration in the Rayleigh–Ritz approximations for the larger eigenvalues, resulting from the use of linear and cubic Hermite functions for the $\{\phi_k\}_{k=1}^n$ is a direct result of their inability to globally approximate the corresponding eigenfunctions (the rate of oscillation of which increases with $k$). It is therefore natural to seek basis functions which do in fact approximate the oscillatory behaviour of the corresponding eigenfunctions. One approach is to take as the $\{\phi_k\}_{k=1}^n$ the (exact) eigenfunctions of a simpler operator which is either similar or semi-similar in the sense of Mikhlin (1976) to the original one (viz. positive definite operators are semi-similar (similar) if their energy spaces (domains) coincide). In essence, this is the basis of the method proposed by Rayleigh (1873).

A partial illustration of the usefulness of this approach has been given by Geller & Stein (1978), who showed that the approximations generated by their variational method (which corresponds to the implementation of a similar operator approach) are superior to those generated by first and second order perturbation methods.

In geophysical contexts, this type of approach has also been applied by Luh (1974) who uses the eigenfunctions of a layered SNREI Earth model, obtained using the Gilbert propagator matrix method, as the basis functions in a study of the effects of rotation and lateral heterogeneity. Though this strategy ensures a well conditioned algebraic eigenvalue problem for the determination of the required eigenvalues, the attainable accuracy of the
resulting approximations will be limited by the form of the approximation chosen for the
eigenfunction.

Although studies of this type show clearly the effectiveness of this approach, convergence
results of the form (2.9) are not in general available. Consequently, the framework proposed
above for the comparison of methods cannot be utilized for the similar operator approach.
However, some measure of its usefulness can be obtained from the result of Mikhlin (1976)
that

$$\lambda_k \leq \lambda_k^{(n)} \leq C \lambda_k, \quad C = C(n) \gg 1, \quad k = 1, 2, \ldots, n.$$ 

It shows that approximate eigenvalues generated in this way have the correct growth as a
function of $k$. In addition, it is clear from the nature of the method that the quality of the
approximation of $\lambda_k$ by $\lambda_k^{(n)}$ will improve as the quality of the approximation of the eigen-
function associated with $\lambda_k$ by $\phi_k$ is improved indicating that uniformly valid approxi-
mations are a possibility.

HA$\text{S}$$\text{K}E$$\text{L}$$\text{L}$ $\text{M}A$$\text{TR}$$\text{I}$$\text{X}$ $\text{M}E$$\text{TH}$$\text{M}$$\text{E}T$h

The essence of Haskell's (1953) matrix method is, with respect to some given partitioning
of $[a, b]$ such as

$$\Delta = \{x_i; \ i = 1, 2, \ldots, n, \quad a = x_0 < x_1 < \ldots < x_n = b\},$$

replace the functions $p, q$ and $r$ of equation (1.1a) by piecewise constant approximations.
The resulting differential eigenvalue problem can be solved in the same manner as a shooting
method, the difference being that the differential equation can now be integrated exactly.
With

$$h = \max_{1 \leq i \leq n-1} |x_{i+1} - x_i|,$$

Pruess (1973) has shown that, under suitable regularity conditions, the following error
estimate holds for general piecewise constant approximations

$$|\lambda_k - \lambda_k^{(n)}| < Ch |\lambda_k|, \quad h < h_0(k). \quad (3.19)$$

If the mid-point rule is used, then

$$|\lambda_k - \lambda_k^{(n)}| < Ch^2 |\lambda_k|^3, \quad h < h_0(k). \quad (3.20)$$

TH$\text{E}$ $P$AINE $\text{A}$ND $D$E HOOG $\text{M}E$$\text{TH}$$\text{M}$$\text{E}T$h

The strategy behind the Paine & de Hoog method (1980) is similar to that of Haskell's
except that equation (1.1a) is first transformed to Liouville normal form before the piece-
wise constant approximation is applied. That is, the Liouville transformation

$$t = T^{-1} \int_a^x (r/p)^{1/2} \, dx, \quad T = \int_a^b (r/p)^{1/2} \, dx,$$

$$u = wz, \quad w = (pr)^{-1/4},$$

under the regularity assumptions

$$p, q, r \in C[a, b], \quad pr \neq 0, \quad pr \in C^2[a, b],$$
is used to transform equation (1.1a–c) to the Liouville normal form

\[- \frac{d^2 z}{dt^2} + sz = T^2 \lambda z, \quad t \in (0, 1)\]

\[
\tilde{a}_1 z(0) + a_2 \frac{dz}{dt}(0) = 0,
\]

\[
\tilde{b}_1 z(1) + b_2 \frac{dz}{dt}(1) = 0,
\]

where

\[
s(t) = [T^2 \left( \frac{q}{r} \right) - \left( \frac{\hat{w}}{w} \right) + 2 \left( \frac{\hat{w}}{w} \right)^2 ](t),
\]

\[
\tilde{a}_1 = a_1 T \left( \frac{p}{r} \right)^{1/2}(a) + a_2 \frac{\hat{w}}{w}(0),
\]

\[
\tilde{b}_1 = b_1 T \left( \frac{p}{r} \right)^{1/2}(b) + b_2 \frac{\hat{w}}{w}(1).
\]

Mathematically, the Sturm–Liouville eigenvalue problem (1.1a–c) is equivalent to the Liouville normal form above in the sense that, except for the constant multiple \(T^2\), their spectra are identical.

The function \(s(t)\) is replaced by a piecewise constant approximation \(s(t)\) and the resulting eigenvalue problem is solved in the same way as in Haskell's method.

The advantage of this method over Haskell's is that the uniform validity of the approximations \(\lambda_k^{(n)}\) can be established. In fact, from Paine & de Hoog (1979), we obtain

\[|\lambda_k - \lambda_k^{(n)}| \leq C h^2, \quad h = 1/n, \quad k = 1, 2, \ldots, n/2,\]  \hspace{1cm} (3.21)

with \(C\) independent of \(k\). The restriction \(k = 1, 2, \ldots, n/2\) imposed on the range of validity of equation (3.21) is easily circumvented. The value of \(n\) is chosen so that a standard asymptotic formula of the type given in Fix (1967) can be applied for \(k > n/2\). The accuracy of the resulting asymptotic eigenvalues will be uniformly \(O(h^2)\), since the accuracy of such asymptotic expansions is \(O(1/k^2)\) and hence \(O(h^2)\) for \(k > n/2\).

**RE DUC T I O N TO L I O U V I L LE N OR M A L F OR M**

At least for some of the methods discussed, the given error estimates is improved if the eigenvalue problem is first transformed to Liouville normal form. Thus, for Haskell's method, since it is equivalent to Paine & de Hoog's for problems in normal form, the given non-uniform bounds (3.19) can be replaced by the uniform bounds (3.21). Similarly, if the scaled and modified Prüfer phase methods, in conjunction with Huen's, are applied to a problem in normal form, the estimates (3.12) and (3.13) are replaced by the uniform error bound

\[|\lambda_k - \lambda_k^{(n)}| \leq C h^2,\]  \hspace{1cm} (3.22)

which is valid for sufficiently small \(h\) and \(4\lambda_k h^2 < \pi^2\).

For the other methods discussed in Section 3, the given error estimates remain unchanged when they are applied to an eigenvalue problem in normal form.

**A SYMPTOTIC F ORM U L A E**

When available and appropriate, asymptotic formulae for the higher harmonics could be used. Their advantage is their simplicity, but they are difficult to use since it is not an easy
Approximation of eigenvalues in geophysics

matter to accurately assess the harmonic beyond which they can replace standard methods. In addition, the standard asymptotic formulae only hold under suitably strong regularity assumptions which often exclude geophysically interesting situations such as rapid and discontinuous changes in properties (cf. Anderssen & Cleary 1973; Lapwood 1975).

4 Comparison of methods and numerical verification

We are now in a position to use the above error estimates to compare the above methods for computing different types of eigenvalues. Initially, however, we distinguish between methods on the basis of whether or not their associated error estimates are uniformly valid; namely, whether or not their error estimates take the form

\[ |\lambda_k - \lambda_k^{(n)}| < Ch^P, \quad p > 0, \quad 1 < k < n, \quad \alpha < 1, \]

(4.1a)

where \( C \) is independent of \( h \) and \( k \). As stressed in Section 2, when a method is used for which the error is relative in nature (namely, takes the form

\[ |\lambda_k - \lambda_k^{(n)}| < Ch^P \lambda_k^q, \quad p > 0, \quad q > 0, \]

(4.1b)

with \( C \) independent of \( h \) and \( k \), the approximations it generates will approximate the smallest eigenvalue with greatest accuracy and this accuracy will deteriorate as the eigenvalues increase in size.

Consequently, if two methods are compared which are equivalent in all respects except that one has the error estimate (4.1a) while the other has the estimate (4.1b) with approximately the same values of \( C \) and \( p \), then the method with the former estimate represents the superior choice. What complicates the choice most is the existence of methods which have an error (4.1b) with \( p \) considerably larger than that which can arise for methods with error of the form (4.1a). For example, compare the error estimate (3.18) for the Rayleigh–Ritz method with \( p = 6 \) with all the uniformly valid estimates listed in Section 3. None of the uniformly valid estimates has a value of \( p \) greater than 2. Thus, methods with uniformly valid error estimates are not optimal, when the fundamental and/or its first few harmonics are all the eigenvalues to be estimated.

We now turn to a more detailed comparison on the basis of the types of eigenvalues to be estimated.

4.1 The fundamental

When only the fundamental is required, any of the methods of Section 3 could be used to generate an accurate estimate. The use of extrapolation in conjunction with a standard finite difference method would be quite efficient. In general, it would yield estimates at least as accurate as those obtained using the Rayleigh–Ritz method with cubic Hermite splines. Because of the simple non-oscillatory form of the fundamental’s eigenfunction, any reasonable shooting method would also yield an accurate estimate. When a reasonable estimate of the eigenfunction is available, the direct evaluation of the Rayleigh quotient can usually be adopted to take advantage of a strategy invented by Rayleigh (1873); namely, use of a first-order accurate estimate of the eigenfunction of an eigenvalue in the direct evaluation of the Rayleigh quotient yields a second-order accurate estimate of that eigenvalue.

4.2 The fundamental and its first few harmonics

When only the first few harmonics as well as the fundamental are all the eigenvalues required, the choice is between the Rayleigh–Ritz method and the scaled or modified Prüfer
phase method. Preference would be given to a Prüfer phase method if computational efficiency were to be maximized, and, because of the $k^5$ term in equation (3.18), to the Rayleigh–Ritz method if accuracy were the goal.

4.3 THE FIRST $m$ EIGENVALUES ACCURATE TO WITHIN A TOLERANCE $\epsilon$

We now examine the problem of finding approximations to the first $m$ eigenvalues $\{\lambda_j^{(n)}\}_{j=1}^m$ which are accurate to within a given tolerance $\epsilon$; viz.

$$|\lambda_j - \lambda_j^{(n)}| < \epsilon, \quad j = 1, 2, \ldots, m. \quad (4.2)$$

To analyse this situation we note that, since $k^5 \sim k^2$, the ratio of the largest to the smallest error over the first $m$ eigenvalues as predicted by equation (4.1b) is $O(m^{-q})$. Therefore, if $m$ is small, any method will be acceptable because the difference between the largest and smallest errors will not be sufficiently great to cause any difficulty in attaining equation (4.2). Consequently, equation (1.1a–c) can be solved numerically as it stands. High-order methods such as Rayleigh–Ritz with a piecewise cubic Hermite basis, shooting methods and the standard Prüfer substitution will be preferable because they yield excellent approximations with minimal effort.

If, however, $m$ compares in size with $n$ then, for those methods with $q > 0$, the largest error will be substantially greater than the smallest. Thus, in order to guarantee that the largest error is bounded by $\epsilon$, an unnecessarily large increase in $n$ will be required.

To make this more precise, let $n_0$ denote the level of partitioning for which the estimate just holds. Then the partitioning required to guarantee that $\lambda_m$ will be approximated to the same tolerance will be $O(m^{2q/p} n_0)$. Clearly, for large $m$, the effect of the relative error is to greatly reduce the importance of the higher order convergence bounds. In fact, if it is necessary to use methods with relative error estimates of the form (4.1b), then the aim should be to choose the method with $q$ minimized. Clearly, the optimal is a method with $q = 0$ which corresponds to a uniform error estimate.

4.4 UNIFORM APPROXIMATIONS TO FIRST $m$ EIGENFREQUENCIES

Next, we examine the problem of obtaining uniform approximations to the first $m$ eigenfrequencies $\gamma_j$ defined by $\lambda_j = \gamma_j^2$. In this situation, it follows that the approximations $\lambda_j^{(n)}$ must satisfy

$$|\lambda_j - \lambda_j^{(n)}| \leq c e \gamma_j^{1/2}, \quad c = \text{const.}, \quad j = 1, 2, \ldots, m, \quad (4.3)$$

if $\lambda_j^{(n)}$ has the same growth as $\lambda_j$. If $m$ is small, then the most important feature of an error estimate is again the order of its convergence. The value of $q$ in equation (4.1b) is of marginal importance. Now, however, as $m$ increases the situation is slightly less critical than when $\lambda_j, j = 1, 2, \ldots, m$, had to be approximated uniformly. If equation (4.1b) is assumed to hold with $p > 0$, then this is reflected in the fact that it is only necessary to increase $n$ if $q > \frac{1}{2}$ and even then the required increase as a function of $m$ is reduced to $n = 0 \ (m^{(2q-1)/p} n_0)$. The integer $n_0$ denotes the level of partitioning for which the estimate (4.3) just holds with $m = 1$. Thus, for large $m$, a method with a uniform error will be preferable to one which has a non-uniform error of the form (4.1b) with $q > \frac{1}{2}$. If $q < \frac{1}{2}$, then the choice cannot be...
made solely on the grounds of the behaviour of the error, but will have to be based on independent numerical considerations.

4.5 Uniform approximations to first \( m \) eigenperiods

Finally, we consider the problem of deriving uniform approximations to the first \( m \) eigenperiods \( \tau_j \) defined by \( \tau_j = 2\pi/\omega_j \). In this situation, it follows that, as long as the required values of \( \tau_j \) are greater than \( 2\varepsilon \), the approximations \( \lambda_j^{(n)} = [\omega_j^{(n)}]^2 \) must satisfy

\[
|\lambda_j^{(n)} - \lambda_j| < c\varepsilon^{3/2}, \quad c = \text{const.}, \quad j = 1, 2, \ldots, m,
\]

if \( \lambda_j^{(n)} \) has the same growth as \( \lambda_j \). Again, if \( m \) is small, then a method with the highest possible order of convergence should be used. Compared with both the previous situations, the effect of increasing \( m \) is greatly reduced. On the one hand, this is reflected in the fact that it is only necessary to increase \( n \) if \( q > \gamma_2 \) and even then the required increase as a function of \( m \) can be reduced to \( n = 0 \) \((m(2q-3)/\pi n_0)\). The integer \( n_0 \) now denotes the level of partitioning for which the estimate (4.4) just holds with \( m = 1 \). On the other hand, if \( q < \gamma_2 \), then the use of either the modified Prüfer method or the Haskell matrix method with piecewise constant approximations will yield uniformly valid approximations or very close approximations to them.

The above conclusions are now verified numerically. We have already shown at the end of Section 2 that the types of difficulty alluded to above do in fact arise in the published geophysical literature.

In order to illustrate further and to provide a more explicit comparison of the methods, we used each of the methods discussed in Section 3 to construct approximations to the first four eigenvalues of

\[
- \{\exp(-x)u'\}' + \exp(2x)u = \lambda \exp(x)u, \quad u(0) = u(1) = 0,
\]

using a uniform partitioning with \( n = 4 \) (except for the finite difference method with \( n = 5 \)).

Although this example is simple and the above choice of \( n \) is such that in some cases it is not sufficiently large to guarantee the validity of the corresponding error bounds, the results as presented in Table 3 are representative of those which are to be expected in practice. They also illustrate clearly the conclusions which were made previously.

If the approximate eigenvalues of Table 3 are used to construct approximate eigenperiods, then the errors given in Table 4 are readily seen to behave in a more uniform fashion than the eigenvalue errors of Table 3. The methods for which their relative error estimates are such that \( q \approx 1.5 \) or less (cf. finite difference methods, the modified Prüfer method, the Haskell matrix method and the Paine & de Hoog) are seen to yield uniform estimates for the eigenperiods.

5 Economic considerations

When economy is the prime consideration in choosing a method, the aim should be to: (a) replace the given differential eigenvalue problem by a simple algebraic one which is easily constructed and solved; and (b) choose the algebraic eigenvalue problem so that an independent and simple estimate of the error between the differential and algebraic eigenvalues can be estimated.
Table 3. Errors in approximate eigenvalues generated by the various methods when applied to the differential eigenvalue problem (4.5).

<table>
<thead>
<tr>
<th>$k$</th>
<th>Exact eigenvalue $\lambda_k$</th>
<th>Finite difference method</th>
<th>Shooting with fourth-order Runge–Kutta</th>
<th>Prüfer</th>
<th>Modified Prüfer</th>
<th>Rayleigh–Ritz</th>
<th>Haskell</th>
<th>Paine &amp; de Hoog</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.1924</td>
<td>0.1153</td>
<td>0.0254</td>
<td>0.0062</td>
<td>0.0000</td>
<td>0.0383</td>
<td>0.1063</td>
<td>0.0359</td>
</tr>
<tr>
<td>2</td>
<td>15.2332</td>
<td>1.8850</td>
<td>0.2951</td>
<td>6.376</td>
<td>0.0023</td>
<td>0.1569</td>
<td>0.1589</td>
<td>0.1219</td>
</tr>
<tr>
<td>3</td>
<td>31.9461</td>
<td>7.3644</td>
<td>8.9696</td>
<td>19.6014</td>
<td>0.0051</td>
<td>0.9629</td>
<td>0.6093</td>
<td>0.0017</td>
</tr>
<tr>
<td>4</td>
<td>55.3451</td>
<td>10.0482</td>
<td>21.5206</td>
<td>40.3648</td>
<td>0.0197</td>
<td>29.5963</td>
<td>1.0630</td>
<td>0.0011</td>
</tr>
</tbody>
</table>

Table 4. Errors in approximate eigenperiods generated by the various methods when applied to the differential eigenvalue problem (4.5).

<table>
<thead>
<tr>
<th>$k$</th>
<th>Exact eigenperiod $\tau_k$</th>
<th>Finite difference method</th>
<th>Shooting with fourth-order Runge–Kutta</th>
<th>Prüfer</th>
<th>Modified Prüfer</th>
<th>Rayleigh–Ritz</th>
<th>Haskell</th>
<th>Paine &amp; de Hoog</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.7574</td>
<td>0.0311</td>
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In this way, approximate eigenvalues are computed by first solving the algebraic system constructed in (a) and then applying the explicit corrections derived in (b). Such a method, based on the application of finite difference methods to Sturm–Liouville problems in Liouville normal form, has been proposed and examined in some detail by Paine et al. (1980).

Because its implementation (but not its analysis) is essentially simple in nature, we give a brief description and discussion. When the coefficients involved are sufficiently smooth, the study of Sturm–Liouville eigenvalue problems, with appropriate boundary conditions, reduces to a study of the canonical Liouville normal form

\[-y'' + qy = \lambda y, \quad y = y(x), \quad y'' = d^2y/dx^2, \quad 0 < x < \pi, \quad \lambda = \lambda(n), \quad y(0) = y(\pi) = 0. \quad (5.1)\]

If, on the grid

\[G = \{x_j: x_j = jh, j = 0, 1, 2, \ldots, n + 1, \quad h = \pi/(n + 1)\}, \]

finite difference approximations are used to replace equations (5.1) and (5.2) by an algebraic eigenvalue problem of order \(n\), viz.

\[Ly = \lambda^{(n)}y, \quad (5.3)\]

then it is well known that the algebraic eigenvalues \(\lambda_1^{(n)}, \lambda_2^{(n)}, \ldots, \lambda_n^{(n)}\) of equation (5.3) only yield satisfactory approximations for the fundamental \(\lambda_1\) and its first few harmonics \(\lambda_2, \lambda_3, \ldots, \lambda_m (m < n)\). For example, if \(q = 0\) and a central difference formula is used to approximate \(-y''\) on \(G\), then the corresponding algebraic eigenvalues are given by

\[\mu_k^{(n)} = 2 \left[1 - \cos kh\right]/h^2, \quad k = 1, 2, \ldots, n. \]

The corresponding error

\[\Sigma_k^{(n)} = \lambda_k - \mu_k^{(n)}, \quad k = 1, 2, \ldots, n, \]

satisfies

\[\Sigma_k^{(n)} = O(k^4 h^2), \]

which clearly illustrates its rapid growth as a function of \(k\).

But, even though the \(\mu_k^{(n)}\) yield poor estimates of the corresponding \(k^2\) (except for \(k < n\)), the error

\[\Sigma_k^{(n)} = k^2 - 2 \left[1 - \cos kh\right]/h^2 \quad (5.4)\]

yields an accurate estimate of the asymptotic behaviour of \(\lambda_k - \lambda_k^{(n)}\), when central differences have been used to approximate \(-y'' + qy\) on \(G\). In fact, Paine et al. (1980) prove that, if the asymptotic error estimate \(\Sigma_k^{(n)}\) is used to correct the algebraic eigenvalues \(\lambda_k^{(n)}\) derived from equations (5.1) and (5.2) for general \(q\), then the resulting approximations \(\lambda_k + \Sigma_k^{(n)}\) yield uniformly valid approximations: viz.

\[|\lambda_k - \lambda_k^{(n)} - \Sigma_k^{(n)}| \lesssim Ckh^2, \quad k \ll an, \quad \alpha < 1. \quad (5.5)\]

For convenience, we introduce the notation \(\lambda_k^{(n)} = \lambda_k^{(n)} + \Sigma_k^{(n)}\).
Table 5. Error in the standard and corrected finite difference eigenvalue estimates for equations (5.6) and (5.7).

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The errors in the standard and corrected eigenvalue estimates for the first 20 eigenvalues of

\[ -y'' + \exp(x)y = \lambda y, \quad y = y(x), \quad y(0) = y(\pi) = 0, \quad (5.6) \]

obtained using central differences to approximate \(-y''\) and \(n = 39\), are given in Table 5. It is clear from these results that the corrected estimates are greatly superior to the original ones. For the standard estimates, the error is obviously in close agreement with the predicted \(k^4\) growth. Also the growth in the error for the corrected estimates appears to be consistent with that predicted by equation (5.5).

To illustrate that the above technique for correcting algebraic eigenvalues does in fact have general applicability, we list in Table 6 for a sequence of values of \(n\) the error in the corrected eigenvalues for the following almost singular problem

\[ -y'' + (x + 0.1)^2y = \lambda y, \quad y = y(x), \quad y(0) = y(\pi) = 0, \quad (5.8) \]

If we consider the errors for a fixed value of \(k\), then it is clear that the predicted second-order convergence of equation (5.5) is obtained as \(h \rightarrow 0\).

6 A comparison of ‘MODE’ with the method of Paine & de Hoog for the evaluation of eigenfrequencies of 1066A and 1066B

From the point of view of published eigenfrequencies and periods of Earth models, the most frequently used program would appear to be Gilbert & Dziewonski’s program MODE. It is
The eigenperiods generated by MODE along with those obtained using the method of Paine & de Hoog are listed in Tables 7–10 for the Earth models 1066A and 1066B. They indicate that:

(i) Relative to the Paine & de Hoog values, MODE consistently underestimates the eigenperiods and overestimates the eigenfrequencies (and associated eigenvalues) (cf. Tables 8 and 10).

(ii) The Paine & de Hoog and MODE values are virtually identical for overtone number \( n \) greater than 2. With respect to a fixed overtone number, the improvement for increasing angular order number \( l \) is either marginal (when \( n = 0, 1 \) and 2) or non-existent (\( n > 2 \)).

(iii) Relative to the observed eigenperiods, the Paine & de Hoog values give slightly closer estimates of the lowest overtone and angular order numbers.
Table 7. Comparison of observed and Paine & de Hoog eigenperiods $n\tau_1$ for model 1066A.

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Table 8. Comparison of Paine & de Hoog and MODE eigenperiods $n\tau_1$ for model 1066A.

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Table 9. Comparison of observed and Paine & de Hoog eigenperiods $n\tau_1$ for model 1066B.

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Table 10. Comparison of Paine & de Hoog and MODE eigenperiods \( nT_l \) for model 1066B.

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From these comparisons, we can draw the following conclusions:

(a) The nature of many eigenvalue methods is such that they tend to either systematically over- or under-estimate the eigenvalues being sought. Thus, an immediate consequence of (i) is that MODE overestimates the eigenvalues of Earth models. Theoretically, it is known that the Paine & de Hoog method does not suffer from this defect. This is borne out by the results of both Tables 7 and 9 which show an oscillatory behaviour in the error between the Paine & de Hoog and the observed values.

(b) An immediate consequence of (ii) and (iii) is that 1066A and 1066B represent a better fit to the observational data than indicated by MODE.

(c) If it were known that the Paine & de Hoog method tended to under- rather than over-estimate, then a consequence of Tables 7 and 9 would be that the observed eigenperiods under- rather than over-estimate the true eigenfrequencies.

Because MODE has been used to compute eigenfrequencies and periods for numerous papers, a comparison of the above type confirms that geophysical inferences based on the use of eigenfrequencies and periods computed using MODE are not invalid because of any numerical shortcomings in the algorithms used in MODE. In addition, it indicates that the Paine & de Hoog method represents an efficient (though equally accurate) alternative to the use of MODE.

7 Recapitulation

From the above discussion, it is clear that, when choosing a numerical method for a given application, the aim is not to choose the one which has the reputation of being the most reliable in some specific sense, but the one which yields approximations which guarantee the highest probability that inferences to be based on them are correct. Thus, when computing modes of free oscillations of Earth models, the choice of method must be based on the geophysical inferences involved. If accurate estimates of the fundamental modes for various angular order numbers are all that are required, then most of the methods discussed above will suffice. Preference would be given to Prüfer phase methods, if computational efficiency were to be maximized, and to Rayleigh–Ritz methods if accuracy were the goal (cf. Birkoff et al. 1966).
If, on the other hand, accurate estimates of a sequence of modes with fixed angular order number are required, which is often the situation in geophysical applications, then the choice of a method which guarantees uniformly valid approximations must be based on the form in which an estimate of the individual modes is required. For example, only the modified Prüfer and the Paine & de Hoog methods should be used when estimates of the eigenfrequencies or their squares are required (cf. Table 3). If estimates of the eigenperiods suffice, then any one of the following methods can be used (cf. Table 4): finite difference, modified Prüfer, Haskell and Paine & de Hoog.

Finally, we note that, if economy is the prime consideration, then a method along the lines of that proposed recently by Paine et al. (1980) should be sought and implemented.

**Acknowledgments**

This paper has benefited from numerous discussions with Frank de Hoog to whom we acknowledge our thanks. Freeman Gilbert’s approval to include in Section 6 a comparison with MODE is gratefully acknowledged.

**References**


Approximation of eigenvalues in geophysics


