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Note

On Shooting Algorithms for Calculating Sturm–Liouville Eigenvalues

In recent years several shooting algorithms have been proposed for estimating the eigenvalues and eigenfunctions of Sturm–Liouville problems, e.g., Adam and Ixaru [1], Dunker and Gordon [5], Mikhailov and Vulchanov [8], and Paine [10]. These have in common that they are based on the idea of approximating the coefficients in the differential equation by step functions for which the resulting problem can be solved "exactly." Earlier discussions of this method, some containing mathematical theory can be found in Datzeff [4], Gordon [7], Canosa and Gomes de Oliviera [3], and Pruess [11]. This note is a response to the paper of Mikhailov and Vulchanov [8] and points out that their solution algorithm can suffer from some numerical problems in certain cases. Many of the cures have been suggested by prior researchers, but as yet, no one has written a code based on approximating the coefficients which incorporates all of these "fixes." The significant advance in [8], an implementation of an algorithm from Wittrick and Williams [14], gives a cheap way of isolating the nth eigenvalue. In theory this allows a robust search for any eigenvalue desired. No prior algorithm contained this feature, a major step toward a robust code for the Sturm–Liouville problem.

Before presenting some of the numerical problems which can arise, it is necessary to state the problem mathematically. Using notation similar to that in [8], we seek nonzero functions $\psi(x, \lambda)$, the eigenfunctions, and constants λ, the eigenvalues, satisfying

$$(p(x)\,\psi')' + (\lambda r(x) - q(x))\,\psi = 0 \qquad a < x < b \tag{1a}$$

$$\alpha_0 \psi(a, \lambda) - \beta_0\, p(a)\,\psi'(a, \lambda) = 0 \tag{1b}$$

$$\alpha_n \psi(b, \lambda) + \beta_n\, p(b)\,\psi'(b, \lambda) = 0, \tag{1c}$$

where $'$ means d/dx. For simplicity, in this note we assume that (1) is regular, i.e., $[a, b]$ is finite, the coefficients $p(x)$, $q(x)$, and $r(x)$ are continuous on $[a, b]$, $p'(x)$ exists and is continuous on $[a, b]$, and $p(x)$ and $r(x)$ are positive on $[a, b]$. Under these assumptions it is known that there is an infinite set of eigenvalue–eigenfunction pairs (λ_k, ψ_k) with λ_0 bounded below and $\lambda_k \to \infty$ as $k \to \infty$.

The basic idea is to replace this problem with another:

$$(\hat{p}(x)\,\hat{\psi}')' + (\hat{\lambda}\hat{r}(x) - \hat{q}(x))\,\hat{\psi} = 0 \tag{2}$$

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with boundary conditions analogous to (1b)–(1c). The new coefficients are chosen so that (2) is simpler to solve than (1). The standard examples have been piecewise constant or piecewise linear functions. As in [8], we concentrate on the step function case. Assume $[a, b]$ has been partitioned into $a = x_0 < x_1 < \cdots < x_n = b$ and let p_k represent the value of $\hat{p}(x)$ in $[x_k, x_{k+1}]$ (q_k and r_k are similarly defined). A reasonable choice for this is $p((x_k + x_{k+1})/2)$. Set $h_k = x_{k+1} - x_k$, $\tau_k = (\hat{\lambda} r_k - q_k)/p_k$, and $\omega_k = \sqrt{|\tau_k|}$. Then on the kth interval

$$\hat{\psi}(x, \hat{\lambda}) = \hat{\psi}(x_k, \lambda)\, F_k(x_{k+1} - x) + \hat{\psi}(x_{k+1}, \lambda)\, F_k(x - x_k), \tag{3}$$

where

$$F_k(t) = \begin{cases} \sin \omega_k t / \sin \omega_k h_k & \tau_k > \varepsilon \\ \sinh \omega_k t / \sinh \omega_k h_k & \tau_k < -\varepsilon \\ \dfrac{t(1 - \tau_k t^2/6 + \tau_k t^4/120)}{h_k(1 - \tau_k h_k^2/6 + \tau_k^4/120)} & |\tau_k| \leqslant \varepsilon \end{cases} \tag{4}$$

for some small $\varepsilon > 0$. The equation for small $|\tau_k|$ is not given in [8], but (4) is numerically safer. There are many ways of characterizing the eigenvalues which lead to stable algorithms, that in [8] is just one. However, since the main difficulty of [8] is the algorithm for computing the eigenfunctions we concentrate on it. The values $\hat{\psi}(x_k, \lambda)$, $k = 0, \ldots, n$, are nontrivial solutions of a homogeneous linear system derived by applying the boundary conditions (1b)–(1c) and the continuity conditions

$$(\hat{p}\hat{\psi}')(x_k^-, \lambda) = (\hat{p}\hat{\psi}')(x_k^+, \lambda) \qquad k = 1, 2, \ldots, n-1. \tag{5}$$

From (3) the continuity equations become

$$\begin{aligned} -p_{k-1} F'_{k-1}(0)\, \hat{\psi}_{k-1} + [p_{k-1} F'_{k-1}(h_{k-1}) + p_k F'_k(h_k)]\, \hat{\psi}_k \\ - p_k F'_k(0)\, \hat{\psi}_{k+1} = 0, \end{aligned} \tag{6}$$

where we have denoted $\hat{\psi}(x_k, \lambda)$ by $\hat{\psi}_k$. The boundary condition (1b) suggests that the eigenfunction should be normalized by

$$\hat{\psi}(a, \lambda) = \beta_0\, p(a) \qquad \text{and} \qquad \hat{\psi}'(a, \lambda) = \alpha_0. \tag{7}$$

But from the representation (3)

$$\hat{\psi}'(a, \lambda) = -F'_0(h_0)\, \hat{\psi}_0 + F'_0(0)\, \hat{\psi}_1$$

so

$$\hat{\psi}_0 = \beta_0\, p(a) \qquad \text{and} \qquad \hat{\psi}_1 = [\alpha_0 + F'_0(h_0)\, \beta_0\, p(a)]/F'_0(0), \tag{8}$$

which yields the following shooting method for the approximate eigenfunction values at the mesh points:

$$\hat{\psi}_{k+1} = \frac{-p_{k-1}F'_{k-1}(0)\,\hat{\psi}_{k-1} + [p_{k-1}F'_{k-1}(h_{k-1}) + p_kF'_k(h_k)]\,\hat{\psi}_k}{p_kF'_k(0)} \tag{9}$$

for $k = 1, 2, ..., n-1$. This is just step 4 of the algorithm for eigenfunction computation in [8]; unfortunately, the recursion can be unstable when $\tau_k < 0$ for many k. For one example of this, consider the radial Schrödinger equation with Morse potential from [9]. In this case $[a, b] = [0, 10]$, $p(x) = 1$, $r(x) = 1$, and

$$q(x) = -D\{1 - [1 - e^{-a(x-x_e)}]^2\} + D,$$

where $D = 188.4355$, $a = 0.711248$, $x_e = 1.9975$, and the boundary conditions are $\psi(0) = \psi(b) = 0$. It can be verified that $\lambda_0 \approx -178.798 + D = 9.637$. But using (9) with a mesh chosen automatically to keep local errors less than 10^{-4} produces the set of values given in Table I (interpolated to a relatively uniform grid) under the heading shooting. Since $\psi(b) = 0$, this is unacceptable. That such behavior is not surprising can be seen by examining the solution to the new problem (2) when $\tau_k < 0$. The solution on the kth interval consists of two components $\exp(-x\sqrt{|\tau_k|})$ and $\exp(+x\sqrt{|\tau_k|})$. In order to choose λ so that $u(b) = 0$ clearly would require the negative exponential to dominate; yet numerically, it is the positive exponential that will dominate, especially for large b, or large n. Mathematically speaking, the decaying exponential solution is unstable for the initial value problem, though it is fine for the two-point boundary value problem. Any initial value (shooting) technique must fail in trying to compute the zeroth eigenfunction for the Morse potential (or any other problem for which $\tau_k < 0$ for many k). Another related problem which can occur (especially on VAX machines which have a relatively small exponent range) is exponent overflow due to the growing exponential component. The value $\phi(b) = 0.247\text{E} + 47$ from Table I would overflow on many machines. Note that here and in Table I, the notation $1.00\text{E} + n$ means 1.00×10^n.

In an attempt to avoid this instability several authors (e.g., [3]) have suggested shooting from the ends into the middle. One computes one solution to the ODE (1a) with initial condition (6), then another solution to (1a) with final value $\beta_n p(b)$ and final slope $-\alpha_n$. These are scaled so that they match up at the midpoint (or some interior point automatically chosen by the integrator), say, with value one. One then iterates on λ until the derivative at the midpoint is continuous. However, this only disguises the instability; it does not avoid it. This is shown by the second column of Table I; while the huge values generated by the regular shooting algorithm are avoided (because of the final scaling), the answers are just as worthless.

Cures for the instability of the initial value problem are well known. Recall that the vector $\Psi := (\hat{\psi}_0, ..., \hat{\psi}_n)$ is a nontrivial solution to a homogeneous linear system (once the correct eigenvalue has been found). Currently, the recommended method

TABLE I

Zeroth Eigenfunction for the Morse Potential

x	Shooting	$\hat{\phi}_0(x)$ by shooting to the middle	Inverse iteration	
			1	15
0.00	0.000	0.000	0.000	0.000
0.50	$0.133E+7$	$0.144E-12$	$0.241E-2$	$0.262E-7$
1.00	$0.818E+10$	$0.339E-8$	$0.660E-2$	$0.155E-2$
1.50	$0.133E+13$	$0.528E-6$	0.233	0.221
2.00	$0.594E+13$	$0.243E-5$	0.978	0.977
3.00	$0.270E+12$	$0.730E-7$	0.054	0.050
4.00	$0.500E+14$	$0.212E-4$	$0.378E-2$	$0.579E-5$
5.00	$0.279E+19$	1.000	$0.313E-2$	$0.695E-10$
6.00	$0.584E+24$	$0.503E-5$	$0.254E-2$	$0.494E-15$
8.00	$0.679E+35$	$0.279E-16$	$0.191E-2$	$0.389E-26$
10.00	$0.247E+47$	0.000	0.000	0.000

for computing such quantities is inverse iteration (Golub and Van Loan [6]). The idea is to start with some initial approximation $\Psi^{[0]}$, e.g., random, then for $j=1, 2, \ldots$ until convergence, solve the linear system with $\Psi^{[j-1]}$ as the right-hand side, the coefficient matrix that of the original homogeneous system, and the solution $\Psi^{[j]}$. This has been used in Pruess [12] and Paine [10], among others. It is necessary to have a good approximation to the eigenvalue in order for this algorithm to produce good results. For the above example, the final columns of Table I headed inverse iteration give the results with $\lambda = -178.800$ after just one iteration and also at the 15th iteration, where the results have converged. Clearly, these numbers (even for the first iteration) are much more satisfactory than simple shooting. It is also a simple matter to avoid the potential overflows in the shooting algorithm for the eigenvalues by some kind of scaling, e.g., see Paine [10] or Dunker and Gordon [5].

If shooting must be used, then it is important that a stable alternative be implemented, for example, the scaled Prüfer transformation found in the code SLEIGN of Bailey, Shampine, and Gordon [2], or the NAG code D02KDF of John Pryce. In either of these, it is critical that the amplitude variable be correctly scaled to avoid the exponential instability.

Another criticism of [8] is that the step size selection algorithm is fairly primitive since it is based on uniform scaling up or down by some arbitrary constant. More efficient automatic procedures for monitoring local errors are available, e.g., [13]. While controlling local errors is straightforward, instability cannot be detected. For the above Morse example the entries in the shooting column did pass a local (relative) error test. A better idea, especially, for two-point boundary value problems, is to use a global error estimate. This is significantly more complicated to implement but should be much more reliable.

One of the chief advantages of the method of approximating the coefficients is that the asymptotic properties of the Sturm–Liouville eigenvalues and eigenfunctions are preserved. This can be taken advantage of in the algorithm for finding initial brackets for $\hat{\lambda}_k$ given by Mikhailov and Vulchanov. Their algorithm (or a variant thereof) is needed for small values of k, but eventually the asymptotic formulas are sufficiently accurate to initialize the search.

One final comment is that the step function approximation is only $\mathcal{O}(h^2)$ accurate. For high accuracy answers a higher order formula would be more efficient. Dunker and Gordon [5] use piecewise linear approximations which are $\mathcal{O}(h^4)$ accurate. Another alternative is to stay with the step functions but use Richardson's h^2-extrapolation to boost the accuracy. It is not immediately evident how the latter can be reliably incorporated into the bracketing process.

In conclusion, the calculation of Sturm–Liouville eigenvalues using shooting methods seems very attractive; however, unless care is taken, there can be serious problems with the eigenfunction calculation.

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