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Finite-Difference Approximations to Singular Sturm-Liouville Eigenvalue Problems

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Abstract. A modification of the central-difference method is given which greatly improves the convergence when applied to a certain class of singular eigenvalue problems, including the Klein-Gordon equation. The singularity given special treatment is at the finite end.

1. Introduction. A common technique for approximating the discrete eigenvalues of Sturm-Liouville eigenvalue problems of the type

$$-d^2y/dx^2 + q(x)y(x) = \lambda y(x), \qquad 0 < x < \infty, \tag{1}$$

with $y(0) = 0$ and $y(x) \longrightarrow 0$ as $x \longrightarrow \infty$, is to replace infinity by some suitably large number $b > 0$ and then treat the problem over the interval $[0, b]$ with the added boundary condition $y(b) = 0$ by using either the central-difference or Numerov finite-difference methods. A discussion of various implementations and applications of these methods can be found in, for example, Cooley [1] and Keller [4]. The purpose of this paper is to give a new finite-difference method for a class of problems with a singularity at the origin that includes the Klein-Gordon equation. We will treat the infinite interval as described above.

In dimensionless form, the Klein-Gordon equation may be written as

$$-d^2y/dx^2 - (2/x + \alpha^2/x^2)y(x) = \lambda y(x). \tag{2}$$

The eigenfunction corresponding to the smallest eigenvalue of (2) behaves like x^β near zero where β satisfies $.5 \leqslant \beta \leqslant 1$ for $0 \leqslant \alpha \leqslant .5$. It is this type of singularity for which we will develop a finite-difference formula. For a discussion of the Klein-Gordon equation and more general singular problems, see Frank, Land and Spector [3]. A generalization of equation (2) can be described as follows. Let $q(x)$ be real-valued and in $C^2(0, \infty)$, i.e. two continuous derivatives, with $q(x) = x^{-2}\Sigma_{m=0}^{\infty} q_m x^m$ on $0 < x < a + \delta$ for some $a, \delta > 0$ and $q_0 \geqslant -1/4$. Let L be the linear operator $Ly = -y'' + qy$ defined in the Hilbert space $L^2(0, \infty)$ with domain $D = \{y\colon y \in C^2(0, \infty), y \text{ and } Ly \in L^2(0, \infty)\}$. Let $p = 1/2 + (q_0 + 1/4)^{1/2}$. For the case $q_0 < 3/4$ we add boundary condition $\lim_{x\to 0}(px^{p-1}y - x^p y') = 0$ to D. The eigenvalue problem is now to find λ real and y in D so that $Ly = \lambda y$. A Frobenius expansion of such an eigenfunction y on $(0, a + \delta)$ shows that $y(x) = a_1x^p + a_2x^{p+1} + a_3x^{p+2} + \cdots$. Thus, we obtain for p not an integer singularities at the origin similar to the Klein-Gordon equation. We additionally assume q behaves at infinity so that such eigenfunctions vanish

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at infinity and have four bounded derivatives on $[a, \infty)$. This would be the case, for example, if we assumed $q(x) = x^{-1}\Sigma_{m=0}^{\infty} q'_m x^{-m}$ for all x sufficiently large. In Section 2 we define a finite-difference method to approximate λ when $Ly = \lambda y$ and y behaves as described. In Section 3 a numerical example is given.

2. **Finite-Difference Method.** Let Δ_n: $0 = x_0 < x_1 < \cdots < x_n = a < \cdots < x_N < x_{N+1}$ be a partition of $(0, x_{N+1})$ with $x_{i+1} - x_i = a/n = h$ for $0 \leqslant i \leqslant N$. Our difference method is a three-point scheme, i.e. we define the difference operator L_h so that $L_h y|_{x_i} = \alpha_i y_{i-1} + \beta_i y_i + \gamma_i y_{i+1}$, where $y_i = y(x_i)$. The development we give is an adaptation of a technique used on the Bessel equation by Dershem [2]. Some essential modifications are required here in the analysis near the origin and in determining an error bound.

For a technical reason to be made clear later, we will consider cases on $p = 1/2 + (q_0 + 1/4)^{1/2}$. If $p < 2$, choose α_i, β_i and γ_i so that for $i = 2, \ldots, n-1$, $(L_h y - Ly)|_{x_i} = 0$ for all functions of the form $y(x) = a_1 x^p + a_2 x^{p+1} + a_3 x^{p+2}$. One finds after solving the resulting three linear equations that

$$\alpha_i = \left(\frac{i}{i-1}\right)^p \cdot \frac{1}{h^2} \cdot \left(-1 + \frac{p}{i}\right),$$

$$\beta_i = \frac{1}{h^2} \cdot \left(2 - \frac{p^2}{i^2} + \frac{p}{i^2}\right) + q(x_i), \tag{3}$$

and

$$\gamma_i = \left(\frac{i}{i+1}\right)^p \cdot \frac{1}{h^2} \cdot \left(-1 - \frac{p}{i}\right).$$

If $2 < p < 3$, define $\rho = p - 1$ and choose α_i, β_i and γ_i so that for $i = 2, \ldots, n-1$, $(L_h y - Ly)|_{x_i} = 0$ for all functions of the form $y(x) = a_1 x^\rho + a_2 x^{\rho+1} + a_3 x^{\rho+2}$. Redefining $p = \rho$, we obtain the same formulas as in (3). For $3 < p < 4$, define $\rho = p - 2$; and proceed as above. For $p > 4$ or an integer, the eigenfunctions are smooth so that the usual central-difference formula is satisfactory. In the remainder of this section, we assume $p < 4$ is not an integer. For $i = n, \ldots, N$ in all cases, the central-difference formula will be used, i.e. $\alpha_i = -1/h^2$, $\beta_i = 2/h^2 + q(x_i)$ and $\gamma_i = -1/h^2$. Note that as i becomes large the coefficients in (3) approach the central-difference coefficients. For $i = 1$, we set $\alpha_1 = 0$ and choose β_1 and γ_1 so that $(L_h y - Ly)|_h = 0$ for all functions of the form $y(x) = a_1(x^p + q_1 x^{p+1}/2p) + a_2 x^{p+2}$ with $p = 1/2 + (1/4 + q_0)^{1/2}$ in all cases. The solution of the resulting two linear equations is

$$\gamma_1 = \frac{-(4p+2)/h^2 - (p+2)(p+1)q_1/2ph + (p+1)q_1/2h}{3 \cdot 2^p + h2^p q_1/p}$$

and

$$\beta_1 = -(p+2)(p+1)/h^2 + q(h) - 2^{p+2}\gamma_1.$$

The difference method is now the following. The eigenvalues of the matrix $A_h = [a_{ij}]_{N \times N}$ with $a_{ii} = \beta_i$, $a_{i,i-1} = \alpha_i$, $a_{i,i+1} = \gamma_i$ and $a_{ij} = 0$ otherwise are computed

and taken as approximations to the eigenvalues of (1). In order to obtain an estimate for the error made in these approximations, we first obtain an estimate for the truncation error.

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$$(L_h y - Ly)|_{x_i} = \begin{cases} O(h^{1+p}), & i = 1, \\ O(h^2), & i \geqslant 2. \end{cases}$$

Proof. The case $i \geqslant n-1$ is standard [4]. For the case $2 \leqslant i \leqslant n-1$, let $v(x) = x^{-p}y(x)$ with p redefined as in the cases treated earlier. Then as v is in $C^4[0, a]$, use Taylor's theorem to expand $v(x)$ about x_i obtaining $v(x) = v_i'(x - x_i) + v_i''(x - x_i)^2/2 + v_i'''(x - x_i)^3/6 + \int_{x_i}^{x}(x - s)^3 v^{(4)}(s)/6\,ds$. $L_h - L$ applied to $x^p(v_i + v_i'(x - x_i) + v_i''(x - x_i)^2/2)$ at x_i gives zero by construction. L applied to $v_i'''(x - x_i)^3 x^p/6 + \int_{x_i}^{x}(x - s)^3 x^p v^{(4)}(s)/6\,ds$ at x_i also gives zero. Now $L_h(x^p \int_{x_i}^{x}(x - s)^3 v^{(4)}(s)ds)|_{x_i} = O(h^2)$ since $|\alpha_i|, |\beta_i| = O(h^{-2})$ and

$$\left| x^p \int_{x_i}^{x}(x - s)^3 v^{(4)}(s)\,ds \right| \leqslant a^p h^4 \cdot \max_{0 \leqslant s \leqslant a} |v^{(4)}(s)|.$$

Direct substitution shows that

$$|L_h(x^p v_i'''(x - x_i)^3/6)|_{x_i}| = (ih)^{p-1} h^2 |v_i'''|p/3 \leqslant a^{p-1} h^2 |v_i'''|p/3.$$

Since $y = x^p v$, this gives the result for $i = 2, \ldots, n-1$. For the case $i = 1$, we observe from the Frobenius expansion of the eigenfunctions that

$$y(x) = a_1(x^p + q_1 x^{p+1}/2p) + a_2 x^{p+2} + a_3 x^{p+3} + \cdots.$$

Using the fact that $(L_h y - Ly)|_h = 0$ for the first two terms of this expansion for y, direct substitution leads to $(L_h y - Ly)|_h = O(h^{1+p})$, completing the proof.

We observe that A_h is not symmetric. However, define the $N \times N$ diagonal matrix $D_h = [d_{ij}]$ for h sufficiently small by $d_{11} = 1$, $d_{jj} = (a_{j-1,j}/a_{j,j-1})^{1/2} \cdot d_{j-1,j-1}$, $j = 2, \ldots, N$, and $d_{ij} = 0$, otherwise. The cases treated earlier on p insure that $(a_{j-1,j}/a_{j,j-1})$ is positive so that the square root can be taken. A direct computation shows that $D_h A_h D_h^{-1}$ is a symmetric matrix. Using Lemma 3 of Dershem [2], one can deduce (or verify directly) the existence of positive constants C_1 and C_2 so that $C_1 \leqslant d_{jj} \leqslant C_2$ for $j = 2, \ldots, N$ and all N.

Now write $L_h y|_{x_j} - \lambda y_j = \tau_j$, $j = 1, \ldots, N$, where $\tau_j = O(h^2)$ for $j = 2, \ldots, N-1$; and $\tau_1 = O(h^{1+p})$, where λ and y are an eigenpair for (1). Since A_h is an $N \times N$ matrix, y_{N+1} has been set to zero, and thus,

$$\tau_N = (y_{N-1} - 2y_N)/h^2 - y''(x_N) = O(h^2 + h^{-2} y(x_{N+1})).$$

In matrix form, the truncation error formulas may be written as $A_h \bar{y} - \lambda \bar{y} = \bar{\tau}$; and so, $(D_h A_h D_h^{-1} - \lambda I) D_h \bar{y} = D_h \bar{\tau}$. We now proceed as in Keller [4] and deduce an error bound. The eigenvalues of A_h and $D_h A_h D_h^{-1}$ are identical. Now if λ is an eigenvalue of A_h, our approximation will be exact. Otherwise, denoting the eigenvalues of A_h by $\{\Lambda_j\}$ and using the Euclidean norm, we have

$$\|D_h\bar{y}\|_2 \leqslant \|(D_hA_hD_h^{-1} - \lambda I)^{-1}\|_2 \cdot \|D_h\bar{\tau}\|_2 \leqslant \max_{\{\Lambda_j\}} \frac{1}{|\Lambda_j - \lambda|} \|D_h\bar{\tau}\|_2,$$

and

$$\min_{\{\Lambda_j\}} |\Lambda_j - \lambda| \leqslant \|D_h\bar{\tau}\|_2/\|D_h\bar{y}\|_2. \tag{4}$$

Using the estimates on the entries of D_h, we have

$$\|D_h\bar{y}\|_2^2 = \sum_{j=1}^{N} d_{jj}^2 y_j^2 \geqslant \sum_{j=1}^{n} d_{jj}^2 y_j^2 \geqslant C_1^2 \frac{n}{a} \sum_{j=1}^{n} y_j^2 a/n.$$

Since y is in D, it follows that

$$\sum_{j=1}^{n} y_j^2 a/n \longrightarrow \int_0^a y^2\,dx \quad \text{as} \quad n \longrightarrow \infty.$$

Thus, for $h = a/n$ sufficiently small, $\|D_h\bar{y}\|_2 \geqslant k_1 n^{1/2}$ for some constant $k_1 > 0$. Now $\|D_h\bar{\tau}\|_2 \leqslant C_2\|\bar{\tau}\|_2 = C_2(\tau_1^2 + \tau_2^2 + \cdots + \tau_N^2)^{1/2} \leqslant C_2(C_3h^{2+2p} + C_4Nh^4 + \tau_N^2)^{1/2}$ for suitably chosen constants $C_3 > 0$ and $C_4 > 0$. Substituting these inequalities into (4), we then have

$$\begin{aligned} \min_{\{\Lambda_j\}} |\Lambda_j - \lambda| &\leqslant \frac{k_2(C_3h^{2+2p} + C_4Nh^4 + \tau_N^2)^{1/2}}{n^{1/2}} \\ &= k_2(C_3h^{3+2p} + C_4ah^4N/n + h\tau_N^2)^{1/2}, \end{aligned} \tag{5}$$

where $k_2 = C_2/k_1$. Taking x_{N+1} sufficiently large so that the $h^{-2}y(x_{N+1})$ component of τ_N is negligible and keeping $x_N = aN/n$ fixed, we have from (5) that some eigenvalue of A_h approximates λ with an error of $O(h^2)$, since $p \geqslant 1/2$. Note that in the case of a finite interval, the method will be exactly $O(h^2)$.

3. **Numerical Example.** We applied the method to the problem $-d^2/dx^2 - (1/4x^2 + 1/x)y = \lambda y$. This corresponds (with a scale change) to $\alpha = 1/2$ in the case of the Klein-Gordon equation. The first eigenvalue can be verified to be $\lambda = -1$ with associated eigenfunction $y(x) = x^{1/2}\exp(-x)$; and in this case, $p = 1/2$. In the following table we give the error made in approximating $\lambda = -1$ and show the effect of varying the point $x = a$, h and x_N. Also, the observed convergence rates are computed, i.e. assuming the error, $e(h)$ behaves like $e(h) = Ch^\beta$, then $\beta = \ln(e(h_1)/e(h_2))/\ln(h_1/h_2)$. In the table $.abc\text{-}d$ denotes $.abc \cdot 10^{-d}$.

TABLE

h	a	x_N	$e(h)$	β	h	a	x_N	$e(h)$	β
1/16	1	12	.985-3	—	1/16	4	12	.800-3	—
1/32	1	12	.270-3	1.87	1/32	4	12	.222-3	1.85
1/64	1	12	.707-4	1.94	1/64	4	12	.582-4	1.93
1/128	1	12	.181-4	1.97	1/128	4	12	.149-4	1.97
1/256	1	12	.457-5	1.98	1/256	4	12	.377-5	1.98
1/384	1	12	.204-5	1.99	1/128	8	12	.149-4	—
1/128	2	12	.151-4	—	1/256	8	12	.377-5	1.98
1/128	1/2	12	.386-4	—	1/128	8	20	.149-4	—

The actual difference between the approximations with $h = 1/128$, $a = 8$ and $x_N = 12$ and $x_N = 20$ was $.48 \cdot 10^{-8}$. Application of the usual central-difference formula with $h = 1/128$ and $x_N = 12$ gave an error of .401 as compared to an error of $.149 \cdot 10^{-4}$ for the new method, and $h = 1/128$, $a = 4$, and $x_N = 12$. This represents an improvement by a factor of approximately 27,000. The error was improved by increasing a from $a = 1$ to $a = 4$. However, one must trade this off against the need to take an increased number of pth-roots. Finally, for $x_N = 8$, the results were affected by the magnitude of $y(x_{N+1})$. With $a = 1$ and $h = 1/128$, an error of $.247 \cdot 10^{-4}$ was observed.

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