Archivum Mathematicum

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Archivum Mathematicum, Vol. 23 (1987), No. 1, 1--8

Persistent URL: http://dml.cz/dmlcz/107271

ARCHIVUM MATHEMATICUM (BRNO)
Vol. 23, No. 1 (1987), 1–8

INITIAL–VALUE METHODS FOR COMPUTING EIGENVALUES OF TWO POINT BOUNDARY VALUE PROBLEM*

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(Received September 2, 1985)

Abstract. We propose second order iterative initial value methods to compute eigenvalues and eigenfunctions of second order boundary value problems. Computational aspects are discussed and several examples are included.

Key words. Initial value methods, eigenvalue problems.

MS Classification. Primary 65L10, Secondary 34B15.

1. INTRODUCTION

One of the pioneer problems in mathematical physics is to find eigenvalues and eigenfunctions of the following boundary value problem

$$y'' + \lambda p(t)\, y = 0, \tag{1.1}$$

$$y(a) = y(b) = 0, \tag{1.2}$$

where $\lambda \in R$ and $p \in C[a, b]$ and $p(t) \geqq 0$ for all $t \in [a, b]$. In section 2, we shall show that the method of complementary functions developed in [2] to solve nonlinear boundary value problems can be applied effectively in an iterative way to compute eigenvalues and eigenfunctions of (1.1), (1.2). The obtained algorithm is of second order and we believe that it reduces the amount of computational work needed in other available variety of methods like symmetric and nonsymmetric finite difference methods [3, 4, 6–8, 11, 12], variational methods [6, 7] and for several other methods see [9, 11–13]. In section 3, we provide λ_n^0 an initial approximation to the nth eigenvalue of (1.1), (1.2). We also discuss the use of initial approximation λ_{n+1}^0 which depends on $\bar{\lambda}_n$ (obtained approximate nth eigenvalue). The superiority of the proposed method and the computational difficulties and their remedies are illustrated by considering several examples in section 4. Finally, we note that the method of adjoints [1, 14] can also be used analogously to find eigenvalues and eigenfunctions of (1.1), (1.2).

* Presented to the Conference EQUADIFF 6, Brno, August 26–30, 1985.

2. FORMULATION OF THE METHOD

We fix the eigenfunctions of (1.1), (1.2) by demanding that $y'(a) = 1$. Then, the boundary value problem (1.1), (1.2) is equivalent to the following first order system

$$\begin{aligned} y_1' &= y_2, \\ y_2' &= -p(t)\, y_1 y_3, \\ y_3' &= 0, \end{aligned} \tag{2.1}$$

$$y_1(a) = y_1(b) = 0, \qquad y_2(a) = 1, \tag{2.2}$$

where $y_3 = \lambda$.

Assume trial value of $y_3(a) = \lambda^0$ and integrate (2.1) with the known and the assumed initial conditions to obtain the solution $y_i(t)$; $i = 1, 2, 3$. Let us consider a nearby solution $y_i(t) + \delta y_i(t)$; $i = 1, 2, 3$ where $\delta y_i(t)$ is the first order correction to $y_1(t)$ to produce the actual solution of (2.1), (2.2). The equations of the nearby solution are

$$\begin{aligned} y_1'(t) + \delta y_1'(t) &= y_2(t) + \delta y_2(t), \\ y_2'(t) + \delta y_2'(t) &= -p(t)\,[y_1(t) + \delta y_1(t)]\,[y_3(t) + \delta y_3(t)], \\ y_3'(t) + \delta y_3'(t) &= 0. \end{aligned} \tag{2.3}$$

From the right side of (2.3) on eliminating the higher order terms, we obtained the variational equations

$$\begin{aligned} \delta y_1'(t) &= \delta y_2(t), \\ \delta y_2'(t) &= -p(t)\,[y_1(t)\,\delta y_3(t) + y_3(t)\,\delta y_1(t)], \\ \delta y_3'(t) &= 0. \end{aligned} \tag{2.4}$$

In a similar way, the boundary conditions for the variational equations are obtained and appear as

$$\delta y_1(a) = 0, \qquad \delta y_1(b) = -[y_1(b)]_{(\mathrm{cal})}, \qquad \delta y_2(a) = 0. \tag{2.5}$$

The solution of the linear boundary value problem (2.4), (2.5) can be written as

$$\delta y_i(t) = -\frac{[y_1(b)]_{(\mathrm{cal})}}{u_1(b)}\, u_i(t); \qquad i = 1, 2, 3, \tag{2.6}$$

wheren $u(t)$ is the solution of the following initial value problem

$$\begin{aligned} u_1' &= u_2, \\ u_2' &= -p(t)\,[y_1(t)\,u_3 + y_3(t)\,u_1], \\ u_3' &= 0, \end{aligned} \tag{2.7}$$

$$u_1(a) = 0, \qquad u_2(a) = 0, \qquad u_3(a) = 1. \tag{2.8}$$

Thus, to find $\delta y_3(t) = -\dfrac{[y_1(b)]_{(\mathrm{cal})}}{u_1(b)}$, we use the fact that $y_3(t) \equiv \lambda^\circ$, $u_3(t) \equiv 1$

and integrate the following initial value problem

$$\begin{aligned} y_1' &= y_2, \\ y_2' &= -\lambda^0 p(t)\, y_1, \\ u_1' &= u_2, \\ u_2' &= -p(t)\,(y_1 + \lambda^0 u_1), \end{aligned} \tag{2.9}$$

$$y_1(a) = 0, \qquad y_2(a) = 1, \qquad u_1(a) = u_2(a) = 0. \tag{2.10}$$

Note that we have interpreted the variation $\delta y_i(t)$; $i = 1, 2, 3$ to be the difference between the true (but unknown) and the calculated solution i.e.

$$\delta y_i(t) = y_{i(\text{true})}(t) - y_{i(\text{cal})}(t). \tag{2.11}$$

However, since (2.4) is only an approximate system, the process of finding the true λ is iterative and terminates only when $\delta y_3(t)$ is sufficiently small (less than preassigned tolerance). Thus, from (2.11) if λ^k the kth approximation to the true λ is known then, λ^{k+1} the $(k+1)$th approximation is obtained by integrating

$$\begin{aligned} [y_1']^{(k)} &= [y_2]^{(k)}, \\ [y_2']^{(k)} &= -\lambda^k p(t)\,[y_1]^{(k)}, \\ [u_1']^{(k)} &= [u_2]^{(k)}, \\ [u_2']^{(k)} &= -p(t)\,([y_1]^{(k)} + \lambda^k [u_1]^{(k)}), \end{aligned} \tag{2.12}$$

$$[y_1(a)]^{(k)} = 0, \qquad [y_2(a)]^{(k)} = 1, \qquad [u_1(a)]^{(k)} = [u_2(a)]^{(k)} = 0 \tag{2.13}$$

and

$$\lambda^{k+1} = \lambda^k - \frac{[y_1(b)]^{(k)}_{(\text{cal})}}{[u_1(b)]^{(k)}}; \qquad k = 0, 1, \ldots. \tag{2.14}$$

The above process (2.12)–(2.14) for computing λ is a realization of Newton's method. This can be shown as for ordinary boundary value problems [2], and hence the convergence is quadratic. Further, since for the computation of λ^{k+2} in (2.12) we need only to replace λ^k by λ^{k+1} and the knowledge of $[y_i(t)]^{(k)}$ or $[u_i(t)]^{(k)}$; $i = 1, 2$ is not required, the method is self-starting. Finally, once λ^k an approximation to λ is known then the corresponding $[y_1(t)]^{(k)}$ provides an approximation to the eigenfunction.

The process (2.12)–(2.14) is a forward method in the sense that each iteration requires the integration of (2.12) from the initial point a to the final point b. If the eigenfunctions of (1.1), (1.2) are fixed by the choice $y'(b) = 1$ then, the backward method appear as (2.12) together with

$$[y_1(b)]^{(k)} = 0, \qquad [y_2(b)]^{(k)} = 1, \qquad [u_1(b)]^{(k)} = [u_2(b)]^{(k)} = 0 \tag{2.15}$$

and

$$\lambda^{k+1} = \lambda^k - \frac{[y_1(a)]^{(k)}}{[u_1(a)]^{(k)}}; \qquad k = 0, 1, \ldots. \tag{2.16}$$

3. INITIAL APPROXIMATION

It is well known [5, 10] that the problem (1.1), (1.2) has an infinite sequence of nonnegative eigenvalues

$$0 \leqq \lambda_1 < \lambda_2 < \ldots < \lambda_n < \ldots$$

and for λ_n there exists a unique (except for a multiplicative constant) eigenfunction $u_n(t)$ which has exactly $n-1$ zeros in (a, b). If $t_i \in (a, b)$, $1 < i < n-1$ denotes the ith zero of $u_n(t)$, then

$$\pi(\lambda_n M)^{-1/2} \leqq t_{i+1} - t_i \leqq \pi(\lambda_n m)^{-1/2}; \qquad i = 0, 1, \ldots, n-1, \tag{3.1}$$

where $M = \max_{a \leqq t \leqq b} p(t)$, $m = \min_{a<t<b} p(t)$, $t_0 = a$ and $t_{n+1} = b$. The proof of the inequality (3.1) requires Sturm's comparison theorem [5, 10]. However, for the sake of completeness we shall give a different proof which seems to be new. For this, we note that the differential equation (1.1) together with the boundary conditions $u_n(t_i) = u_n(t_{i+1}) = 0$ is equivalent to the following integral equation

$$u_n(t) = \lambda_n \int_{t_i}^{t_{i+1}} g(t, s)\, p(s)\, u_n(s)\, \mathrm{d}s, \tag{3.2}$$

where $g(t, s)$ is the Green's function of the problem $-u_n'' = 0$, $u_n(t_i) = u_n(t_{i+1}) = 0$ i.e.

$$g(t, s) = \frac{1}{(t_{i+1} - t_i)} \begin{cases} (s - t_i)(t_{i+1} - t), & t_i \leqq s \leqq t \leqq t_{i+1}, \\ (t - t_i)(t_{i+1} - s), & t_i \leqq s \leqq t \leqq t_{i+1}. \end{cases}$$

Without loss of generality we assume that $u_n(t) > 0$ in (t_i, t_{i+1}) then, the function $\varphi_i(t) = \dfrac{u_n(t)}{\sin \dfrac{\pi(t - t_i)}{(t_{i+1} - t_i)}}$ is well defined on $[t_i, t_{i+1}]$ and $0 < k_i = \min_{t_i \leqq t \leqq t_{i+1}} \varphi_i(t) \leqq$ $\leqq \max_{t_i \leqq t \leqq t_{i+1}} \varphi_i(t) = K_i$. Thus, from (3.2) we find

$$\varphi_i(t) = \frac{\lambda_n}{\sin \dfrac{\pi(t - t_i)}{(t_{i+1} - t_i)}} \int_{t_i}^{t_{i+1}} g(t, s)\, p(s) \sin \frac{\pi(s - t_i)}{(t_{i+1} - t_i)}\, \varphi_i(s)\, \mathrm{d}s$$

and hence

$$\frac{\lambda_n}{\sin \dfrac{\pi(t - t_i)}{(t_{i+1} - t_i)}} m k_i \int_{t_i}^{t_{i+1}} g(t, s) \sin \frac{\pi(s - t_i)}{(t_{i+1} - t_i)} \leqq \varphi_i(t) \leqq$$

$$\leqq \frac{\lambda_n}{\sin \dfrac{\pi(t - t_i)}{(t_{i+1} - t_i)}} M K_i \int_{t_i}^{t_{i+1}} g(t, s) \sin \frac{\pi(s - t_i)}{(t_{i+1} - t_i)}\, \mathrm{d}s. \tag{3.3}$$

However, since

$$\int_{t_i}^{t_{i+1}} g(t, s) \sin \frac{\pi(s - t_i)}{(t_{i+1} - t_i)} \, ds = \frac{(t_{i+1} - t_i)^2}{\pi^2} \sin \frac{\pi(t - t_i)}{(t_{i+1} - t_i)},$$

the inequality (3.3) is same as

$$\lambda_n m k_i \frac{(t_{i+1} - t_i)^2}{\pi^2} \leqq \varphi_i(t) \leqq \lambda_n M K_i \frac{(t_{i+1} - t_i)^2}{\pi^2}. \tag{3.4}$$

Since (3.4) is true for all $t \in [t_i, t_{i+1}]$, in particular we find that

$$\lambda_n m \frac{(t_{i+1} - t_i)^2}{\pi^2} \leqq 1 \leqq \lambda_n M \frac{(t_{i+1} - t_i)}{\pi^2},$$

which is same as (3.1).

Now, from (3.1) we have

$$n\pi(\lambda_n M)^{-1/2} \leqq \sum_{i=0}^{n-1} (t_{i+1} - t_i) = b - a \leqq n\pi(\lambda_n m)^{-1/2}$$

and hence

$$\frac{n^2\pi^2}{M(b - a)^2} \leqq \lambda_n \leqq \frac{n^2\pi^2}{m(b - a)^2} \tag{3.5}$$

in which the equality holds if $p(t)$ is a constant.

From the inequality (3.5), we find that $\dfrac{n^2\pi^2}{M(b - a)^2}$ or $\dfrac{n^2\pi^2}{m(b - a)^2}$ or $\dfrac{1}{2} \dfrac{n^2\pi^2}{(b - a)^2} \left[\dfrac{1}{M} + \dfrac{1}{m}\right]$ can be taken as an initial approximation λ_n^0 to λ_n the nth eigenvalue of (1.1), (1.2). However, in practical applications m may be zero, in which case the last two initial approximations are not obtainable. Difficulties also arise in using all these approximations for $n > 1$. This is due to the fact that the lower bound may be closer to, or even less than the next smaller eigenvalue namely λ_{n-1} then, the iteration process (2.12)–(2.14) is likely to converge to λ_{n-1} instead of λ_n. Similarly, when $m \neq 0$, the use of the upper bound may lead to convergence to λ_{n+1} instead of λ_n.

The modify the choice of the initial approximation for $n > 1$, we note that $\lambda_n = \dfrac{n^2\pi^2}{\mu_n(b - a)^2}$ and $\lambda_{n+1} = \dfrac{(n + 1)^2\pi^2}{\mu_{n+1}(b - a)^2}$ where $m \leqq \mu_n, \ \mu_{n+1} \leqq M$. Thus, $\dfrac{\lambda_{n+1}}{\lambda_n} = \dfrac{(n + 1)^2}{n^2} \dfrac{\mu_n}{\mu_{n+1}}$. If the variation of $p(t)$ is small in $[a, b]$, we can say $\dfrac{\mu_n}{\mu_{n+1}} \cong 1$. Hence $\lambda_{n+1} \cong \dfrac{(n + 1)^2}{n^2} \lambda_n$ i.e. for the computation of λ_{n+1} we can

take $\frac{(n+1)^2}{n^2}\lambda_n$ as an initial approximation. The disadvantage here is that intermediate eigenvalues have to be found before higher ones. But an initial approximation with $\frac{(n+k)^2}{n^2}\lambda_n$ for the computation of $\lambda_{n+k}(k \geqq 1)$ improves as n increases, so we need only very rough estimates of intermediate eigenvalues.

4. NUMERICAL COMPUTATION

A simple Fortran routine using fourth-order Runge-Kutta method is implemented on IBM 3081 GX. The computation was applied for the first eigenvalue λ_1 to several test functions $p(t)$ and different choices of a and b, however to obtain convergence to seven or eight significant figures the number of iterations is too large e.g. let $p(t) = 1$, $a = 0$, $b = 1$ for which $\lambda_1 = \pi^2$, if $\lambda^\circ = 8$ then, with $h = 0.1, 0.01, 0.001$ or $0.000\,1$ it requires 160 to 200 iterations each. An extrapolation routine was then included in the algorithm to accelerate the convergence. The scheme known as Aitken's extrapolation formula is as follows. Let λ° denote the initial approximation, and λ^1, λ^2 denote the successive iterated approximations using (2.14) or (2.16) then, we compute

$$\bar{\lambda} = \frac{(\lambda^0\lambda^2 - (\lambda^1)^2)}{(\lambda^2 - 2\lambda^1 + \lambda^0)}.$$

This $\bar{\lambda}$ is used as the next initial approximation.

We apply this procedure to test functions (i) $t(1-t)$, (ii) $\sin t$, (iii) $\cosh t$, (iv) $1 + t^2$ with $a = 0$, $b = 1$. Table 1 displays the results of computation of λ_1 with their initial approximations, step size and (n, m) where n is the number of iterations and m the extrapolations needed to achieve the convergence. Table 2 displays the first five eigenvalues of each together with their initial approximations. The convergence to ten significant figures is achieved with 10 iterations and 4 extrapolations.

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Table 1

$p(t)$	λ_1^0	$h = 0.1$		$h = 0.01$		$h = 0.001$		$h = 0.000\,1$	
		(n, m)	α	(n, m)	α	(n, m)	α	(n, m)	α
$t(1-t)$	$4\pi^2$	(12,5)	45.855 055 37	(10,4)	45.250 172 44	(10,4)	45.244 264 90	(8,3)	45.244 205 83
$\sin t$	$\frac{\pi^2}{\sin 1}$	(10,4)	18.685 848 66	(10,4)	20.054 941 64	(10,4)	20.205 901 45	(10,4)	20.221 145 76
$\cosh t$	$\frac{\pi^2}{\cosh 1}$	(10,4)	8.380 873 33	(10,4)	8.570 386 58	(10,4)	8.588 649 94	(10,4)	8.590 467 68
$1 + t^2$	$\frac{\pi^2}{2}$	(10,4)	7.333 627 50	(10,4)	7.612 410 91	(10,4)	7.639 840 30	(10,4)	7.642 576 51

Table 2. $h = 0.000\,01$

$p(t)$	λ_1		λ_2		λ_3		λ_4		λ_0	
	λ_1^0		$\lambda_2^0 \cong \cong 4\lambda_1$		$\lambda_3^0 \cong \cong \frac{9}{4}\lambda_2$		$\lambda_4^0 \cong \cong \frac{16}{9}\lambda_3$		$\lambda_5^0 \cong \cong \frac{25}{16}\lambda_4$	
$t(1-t)$	$4\pi^2$	45.244 205 25	181.00	215.771 465 9	485.5	514.356 517 3	914.4	940.970 043 0	1 475.0	1 495.598 597 4
$\sin t$	$\frac{\pi^2}{\sin 1}$	20.222 671 69	80.67	87.856 297 83	197.7	203.235 387 0	361.6	366.361 631 0	572.4	577.234 498 5
$\cosh t$	$\frac{\pi^2}{\cosh 1}$	8.590 649 361	34.36	33.898 317 30	76.27	76.077 256 25	135.2	125.128 290 5	211.1	211.051 195 9
$1 + t^2$	$\frac{\pi^2}{2}$	7.642 850 063	30.57	30.245 656 36	67.83	67.603 771 40	120.2	120.044 367 9	187.6	187.468 083 9

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