Inclusion of eigenvalues and eigenfunctions of the Sturm–Liouville problem

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Abstract

We compute verified inclusions of eigenvalues and eigenfunctions of the Sturm-Liouville equation. The bounds are calculated on a computer. Using machine interval arithmetic, all truncation and rounding errors are enclosed.

1. INTRODUCTION

We consider the Sturm–Liouville boundary value problem

$$\begin{aligned} -u'' + q(x)\,u &= \lambda\,u \quad , \quad x \in [\,0\,,\,\pi\,] \\ u(0) &= u(\pi) = 0 \end{aligned} \tag{1}$$

where $q(x)$ is a continuous function in $[\,0\,,\,\pi\,]$ and λ a real parameter. λ is called an eigenvalue of (1), if there exists a non–trivial solution $u(x)$. In this case $u(x)$ is called an eigenfunction of (1).

In the following we state some well–known results about (1) that can be found in any standard text book on ordinary differential equations (see Walter [5], for example). The first is about existence of eigenvalues:

Theorem 1: Under the above assumptions on $q(x)$, (1) has an infinite number of (simple) eigenvalues $\lambda_0 < \lambda_1 < \lambda_2 < \ldots$, that tend to infinity. A corresponding eigenfunction $u_n(x)$ has exactly n zeroes in $(\,0\,,\,\pi\,)$.

Now consider the following initial value problem for $u = u(x,\mu)$:

$$\begin{aligned} -u'' + q(x)\,u &= \mu\,u \quad , \quad x \in [\,0\,,\,\pi\,] \\ u(0) &= 0 \quad , \quad u'(0) = 1 \end{aligned} \tag{2}$$

(2) has a unique solution $u(x,\mu)$ for every $\mu \in \mathbb{R}$ and μ is equal to an eigenvalue λ_n, $n \in \mathbb{N}_0$, of (1), iff $u(\pi,\mu) = 0$. Counting the zeroes of $u(x,\mu)$ in $(\,0\,,\,\pi\,]$ we get lower and upper bounds of eigenvalues of (1) from

Theorem 2: Let $u(x,\mu)$ be a solution of (2) for a given $\mu \in \mathbb{R}$. Denote by $N(\mu)$ the number of zeroes of $u(x,\mu)$ in $(\,0\,,\,\pi\,]$ and let $\lambda_{-1} := -\infty$. Then $N(\mu)$ is an increasing function of μ and $\lambda_{N(\mu)-1} \le \mu < \lambda_{N(\mu)}$.

Corollary 1: For $\lambda = \lambda^-,\ \lambda^+$ with $N(\lambda^-) \le n$, $N(\lambda^+) \ge n+1$ it holds that $\lambda^- < \lambda_n \le \lambda^+$.

The next theorem will be needed in chapter 4 to derive approximations of eigenvalue bounds:

Theorem 3: The Sturm–Liouville problem is monotone in $q(x)$, that is if $p(x) \le q(x)$ for all $x \in [\,0\,,\,\pi\,]$ then $\lambda_n(\,p(x)\,) \le \lambda_n(\,q(x)\,)$ for all $n \in \mathbb{N}_0$.

2. INCLUSION OF EIGENVALUES

Suppose we solve (2) for two numbers λ^- , λ^+ satisfying the assumptions of corollary 1. Then we have an immediate but presumably rough inclusion of the n–th eigenvalue λ_n of (1) . Note that we obtain an inclusion of λ_n without knowledge of the other eigenvalues of (1) .

To improve given bounds of λ_n we solve (2) for some $\mu \in [\,\lambda^-\,,\,\lambda^+\,]$ and apply corollary 1 to λ^- and μ or μ and λ^+ . If we are close enough to λ_n , that is if $N(\lambda^-) = n$ and $N(\lambda^+) = n+1$, then convergence speed is improved be applying the regula falsi (or any other method suited to compute inclusions of simple zeroes of a real–valued function) to $f(\mu) := u(\pi,\mu)$.

Usually, computing bounds in every iteration step is a slow process and we can speed up convergence considerably if we first compute a good approximation λ^* of λ_n by a

fast method (using real machine arithmetic) and then derive bounds λ^- and λ^+ adding or substracting a suitable number ϵ .

When applying the secant method we have to solve one (ivp) in every iteration step (the same amount of work is due for bisection of $[\lambda^-, \lambda^+]$ or the regula falsi method). Newton's method requires the computation of $f'(\mu)$, where

$$f'(\mu) = u_\mu(\pi,\mu) = \frac{\partial}{\partial\mu}(u(x,\mu))\Big|_{x=\pi}$$

and $v(x,\mu) := u_\mu(x,\mu)$ satisfies

$$-v'' + q(x)\, v = \mu\, v + u \;, \quad v(0) = v'(0) = 0 \;.$$

In this case we have to solve two (ivp) per iteration.

3. PRÜFER TRANSFORMATION OF (2)

There is an alternative approach to solve (2) applying the Prüfer transformation. Introducing polar coordinates

$$u'(x) =: \rho(x) \cos\phi(x) \;, \quad u(x) =: \rho(x) \sin\phi(x)$$

in the phase plane $(u'(x), u(x))$, and inserting these into (2) we get two first order equations for ϕ and ρ :

$$\phi'(x) = (\lambda - 1 - q(x)) \sin^2\phi + 1 \;, \quad \phi(0) = 0 \tag{3}$$

$$\rho'(x) = (1 - \lambda + q(x))\, \rho \cos\phi \sin\phi \;, \quad \rho(0) = 1 \;. \tag{4}$$

The following theorem holds:

Theorem 4 : a) $\lambda = \lambda_n \;\Leftrightarrow\; \phi(\pi,\lambda) = (n+1)\,\pi \;, \quad n \in \mathbb{N}_0 \;.$

b) $\phi_\lambda(\pi,\lambda) = \frac{\partial}{\partial\lambda}(\phi(x,\lambda))\Big|_{x=\pi} > 0$ for all $\lambda \in \mathbb{R}$.

Note that we do not have to solve (4) to obtain eigenvalue inclusions. $\rho(x)$ is only needed to compute eigenfunctions of (1). As (4) is a linear first order equation for ρ, it can be solved by quadrature, after (3) has been solved.

All methods described in chapter 2 apply to the transformed problem (3), where

$$g(\mu) := \phi(\pi,\mu) - (n+1)\,\pi$$

instead of $f(\mu)$ is used. But there is a considerable simplification of Newton's method. The derivative $g'(\mu)$ can be computed without solving an initial value problem, that is $g'(\mu) = \phi_\mu(\pi,\mu)$, where $\Psi(x,\mu) := \phi_\mu(x,\mu)$ satisfies

$$\Psi'(x) = (\lambda - 1 - q(x))\sin(2\phi)\,\Psi + \sin^2\phi\,, \quad \Psi(0) = 0\,.$$

This is a linear first order equation for Ψ that can be solved by quadrature. Therefore, in this case, we have to solve only one initial value problem in each Newton step.

4. INTERVAL INCLUSION $[u](x,\mu)$ OF $u(x,\mu)$

In applications we will not be able to solve the initial value problem (2) explicitly. But if we only compute approximate solutions $u^*(x,\mu)$ to $u(x,\mu)$, we can not guarantee that $u^*(x,\mu)$ and $u(x,\mu)$ have the same number of zeroes in $(0, \pi]$. Therefore we have to solve (1) with an interval method (see [1]), that computes an inclusion

$$[u](x,\mu) = [\,lb(u(x,\mu)),\ ub(u(x,\mu))\,]$$

of $u(x,\mu)$.

Now suppose that $[u(x,\mu)]$ has n zeroes in $(0, \pi)$. Then μ is a guaranteed upper bound of the (n–1)–th eigenvalue of (2). It is a guaranteed lower bound of λ_n, if $0 \notin [u(\pi,\mu)]$. No decision about a lower bound can be made in the case $0 \in [u(\pi,\mu)]$, as $N(u(x,\mu))$ could be equal to either n or n+1, depending on the function value $u(\pi,\mu) \in [u(\pi,\mu)]$.

Counting the zeroes of $[u](x,\mu)$ one has to make sure that if $[u](x,\mu)$ crosses the real axis, the true solution $u(x,\mu) \in [u](x,\mu)$ has only one zeroe there. This can be guaranteed if we compute an inclusion $[u'](x,\mu)$ of $u'(x,\mu)$ as well and if for every $x \in [0, \pi]$ with $0 \in [u](x,\mu)$ it holds that $0 \notin [u'](x,\mu)$.

5. INITIAL APPROXIMATIONS

As we have seen in chapters 2 and 3 , improving eigenvalue bounds is – theoretically – a simple task. Deriving good, reliable and easy–to–find initial approximations for the eigenvalues proves to be more difficult. We state three well–known possible ways to proceed.

First, due to theorem 3 there is the immediate estimate

$$| \lambda_n - (1+n)^2 | \leq \| q \|_\infty ,$$

as $\lambda_n = (n+1)^2$ for $q(x) \equiv 0$.

Secondly, if $q(x)$ is smooth enough there is an asymptotic expansion of eigenvalues due to Fix [2] :

$$\sqrt{\lambda_{n-1}} = n + \frac{1}{2n} Q_1 + \frac{1}{8n^3} (Q_2 - Q_1^2 + q'(\pi) - q'(0)) + O(\frac{1}{n^4})$$

$$\text{where} \quad Q_1 = \frac{1}{\pi} \int_0^\pi q(x)\, dx \ , \quad Q_2 = \frac{1}{\pi} \| q(x) - Q_1 \|_2^2 \quad .$$

Thirdly, the standard Rayleigh–Ritz method will supply upper bounds for the eigenvalues, that can be used as eigenvalue approximations as well.

Eigenvalue expansions only lead to good approximations if Q_1 and Q_2 are small. Likewise, the bounds given by the infinity norm are only usefull when the latter is small. In most cases the Rayleigh–Ritz method is likely to produce the best results. But note that it will not supply lower bounds of the eigenvalues.

6. INCLUSION OF EIGENFUNCTIONS

To compute eigenvalue inclusions in chapter 4 we had to have an interval solver for (2) , that is we had to compute interval inclusions $[u] (x,\mu)$ of solutions $u(x,\mu)$ of (2) , for all $x \in [0 , \pi]$ and $\lambda \in \mathbb{R}$. Extending our solver to interval input for μ, we compute inclusions $[u] (x,[\mu^-,\mu^+])$ of solutions $u(x,\mu)$ of (2) so that

$u(x,\mu) \in [u] (x,[\mu^-,\mu^+])$ for all $x \in [0 , \pi]$ and all $\mu \in [\mu^- , \mu^+]$.

Now we obtain eigenfunction inclusions of (1) in two steps. First we compute an inclusion $[\lambda^-, \lambda^+]$ of the n–th eigenvalue λ_n of (1). Secondly we enclose the normalized n–th eigenfunction $u_n(x)$ via

$$u_n(x) = u(x,\lambda_n) \in [u](x,[\lambda^-,\lambda^+]) \text{ for all } x \in [0, \pi].$$

7. NUMERICAL RESULTS

We used the algorithm AWA by Lohner [4] to solve (2). All computations were performed on an HP Vectra (386–20) computer under PASCAL–XSC (see [3]). All discretation and rounding errors were taken into account.

To compute the Rayleigh–Ritz approximations, the symmetry of q(x) (and of the eigenfunctions) was utilized to split the matrix eigenvalue problem into two problems for the even and the odd eigenvalues, respectively. The standard trial functions $\sin(jx)$, $j = 1, 2, \ldots$ were used.

In the following tables we show verified inclusions of eigenvalues compared to Rayleigh–Ritz approximations and approximations by asymptotic formulae. The latter are only shown where they lead to reasonable results.

Example I (Mathieu–equation) : Eigenvalues of $q(x) = \cos(2x)$

Nr. of Taylor – coefficients in AWA : 15 Step size : $h = \pi / 90$
Nr. of trial functions for the Rayleigh – Ritz method : 20

n	asympt. exp.	Rayleigh–Ritz	interval inclusion of λ_n
0	1.125 000	0.470 654	$0.470\ 654\ 354\ 933\ 8\frac{45}{32}$
1	4.041 250	3.979 188	$3.979\ 189\ 215\ 751\ 3\frac{72}{42}$
2	9.013 888	9.013 719	$9.013\ 719\ 838\ 920\ \frac{416}{367}$
10	121.001 033	121.001 042	$121.001\ 041\ 672\ 5\frac{800}{779}$

Example II : Eigenvalues of $q(x) = 1000 \cos(2x)$

Nr. of Taylor – coefficients in AWA : 15 Step size : $h = \pi / 1000$
Nr. of trial functions for the Rayleigh – Ritz method : 60

n	Rayleigh–Ritz	interval inclusion of λ_n
0	–955. 530 062	$-955.\ 530\ 062\ 027\ 49^{68}_{28}$
1	–867. 098 865	$-867.\ 098\ 865\ 357\ 0^{542}_{479}$
2	–779. 694 176	$-779.\ 694\ 175\ 891\ ^{9070}_{8999}$
10	–119. 964 807	$-119.\ 964\ 806\ 058\ 9^{909}_{780}$

Example III : Eigenvalues of $q(x) = 1000 \cos(2000x)$

Nr. of Taylor – coefficients in AWA : 15 Step size : $h = \pi / 4000$

n	interval inclusion of λ_n
0	$0.87^{4\ 998}_{5\ 002}$
1	$3.87^{4\ 995}_{5\ 004}$
2	$8.87^{4\ 992}_{5\ 006}$
10	$120.87^{4\ 962}_{5\ 008}$

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