

Enclosing solutions of an inverse Sturm-Liouville problem with finite data

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Abstract — Zusammenfassung

Enclosing solutions of an inverse Sturm-Liouville problem with finite data.

This paper is concerned with the reconstruction of an unknown potential $q(x)$ in the Sturm-Liouville problem with Dirichlet boundary conditions, when only a finite number of eigenvalues are known. The problem is transformed into a system of nonlinear equations. A solution of this system is enclosed in an interval vector by an interval Newton's method. From the interval vector, an interval function $[q](x)$ is constructed that encloses a potential $q(x)$ corresponding to the prescribed eigenvalues. To make this numerical existence proof rigorous, of course, all discretization and rounding errors have to be taken into account in the computation.

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Lösungseinschließung eines inversen Sturm-Liouville-Problems mit endlichen Daten. In dieser Arbeit wird die Rekonstruktion eines unbekanntes Potentials $q(x)$ im Sturm-Liouville-Problem mit Dirichletschen Randbedingungen behandelt, wobei nur endlich viele Eigenwerte als bekannt vorausgesetzt werden. Dieses Problem wird in ein nichtlineares Gleichungssystem überführt. Mit einem Intervall-Newtonverfahren wird eine Lösung des Gleichungssystems in einen Intervallvektor eingeschlossen. Aus dem Intervallvektor wird eine Intervallfunktion $[q](x)$ konstruiert, die ein Potential $q(x)$ einschließt, das die gestellte Rekonstruktionsaufgabe löst. Um auf diese Weise den numerischen Existenznachweis einer Lösung zu führen, sind die bei der praktischen Berechnung auftretenden Diskretisierungs- und Rundungsfehler zu berücksichtigen.

1 Introduction

Consider the Sturm-Liouville problem with Dirichlet boundary conditions:

$$\begin{aligned} -u'' + q(x)u &= \lambda u \\ u(0) &= u(\pi) = 0. \end{aligned} \tag{1}$$

In this paper, $q(x)$ is assumed to be a continuous function in $[0, \pi]$, symmetric about $\frac{\pi}{2}$, that is $q(x) = q(\pi - x)$ for all $x \in [0, \pi]$. A real number λ is called an eigenvalue of (1) if there is a nontrivial solution $u(x)$ of the boundary value problem (1). In this case, $u(x)$ is called an *eigenfunction* of (1). The set of all eigenvalues is the *spectrum* of (1). As is well known, the spectrum of (1) is an infinite sequence of real numbers which is bounded from below and tends to infinity ([23], Theorem 2.1). As in [23], we refer to (1) as *Dirichlet problem* and regard eigenvalues of (1) as functionals of $q(x)$, denoted by $\lambda_i(q)$, $i \in \mathbb{N}$, where the $\lambda_i(q)$ are ordered increasingly:

$$\lambda_1(q) < \lambda_2(q) < \dots .$$

The opposite of the computation of eigenvalues and eigenfunctions of (1) for a given potential $q(x)$, the *inverse Dirichlet problem* is concerned with the reconstruction of $q(x)$ in (1) from spectral data. In his fundamental paper in 1946, Borg [6] proved that there exists a symmetric potential $q(x)$ corresponding to a given spectrum if the eigenvalues satisfy certain asymptotic expansions, and that a symmetric potential is uniquely defined by all eigenvalues of (1). The first numerical scheme was originated by Gel'fand and Levitan [7] in 1951. Since then, several reconstruction procedures have been suggested (cf. [4], [5], [8], [12], [17], [18], [24], [25]; further references are given in [8] and [17]).

A crucial property of the inverse problem is the fact that *all* eigenvalues are needed to determine the potential uniquely, whereas in applications only a relatively small number of the lowest eigenvalues can be measured. Two principal methods have been developed to deal with this inconsistency.

The first method – originated by Gel'fand and Levitan [7] – works with an auxiliary potential $\tilde{q}(x)$, from which the higher eigenvalues are taken. The completed spectrum then defines exactly one potential $q(x)$, and the only (though still difficult) remaining problem is the actual computation of q . However, the choice of the auxiliary potential \tilde{q} is arbitrary; a small variation on \tilde{q} (measured in the infinity norm) may result in a large variation on q .

In the second approach, one tries to reconstruct a potential in a given function set S from finitely many eigenvalues ([5], [11], [17]). In applications, additional information on properties of the solution (eg. smoothness, monotonicity or periodicity) can be incorporated into the choice of S . However, for a given number of n eigenvalues and a given function set S , it may neither be possible to decide whether a solution exists in S nor whether it is uniquely defined in S . A different choice of S may result in a different potential q , or in no solution at all.

A representation of the difference between any two potentials with the same n lowest eigenvalues has been given by Hochstadt [12] and Hald [10] in the form of a series of functions whose frequency is at least n . Hence, qualitatively speaking, the lowest eigenvalues determine the low frequency modes of the potential, whereas the high frequency modes remain undetermined. A popular approach is to assume a finite trigonometric expansion of $q(x)$ and recover the Fourier coefficients from the given eigenvalues ([11], [17]).

Some of the reconstruction procedures developed so far (e.g. [18]) construct an approximate solution of the inverse Dirichlet problem (that is a function, whose eigenvalues approximate but are not equal to the prescribed eigenvalues). Others ([5], [17]) require an infinite iteration to compute a solution. In addition, to prove the existence of a solution and the convergence of the iteration, the unknown potential may have to be sufficiently small.

When developing a new reconstruction scheme, one of our goals was a precise error estimation in the infinity norm, bounding both the errors committed by the termination of an infinite iteration and roundoff errors in the calculations and in the representation of numbers and functions on a computer. In finitely many iterations, we construct bounds of a solution of the inverse Dirichlet problem (in a given function set S), without an *a priori*-restriction on the infinity norm of q .

The inverse problem is transformed into a system of nonlinear equations. Applying interval Newton's method to this system, we validate the existence and local uniqueness of a solution of the system. We enclose this solution in an interval vector, with which we construct an interval function $[q](x)$ that encloses a solution $q(x)$ of the inverse Dirichlet problem.

A more detailed description of some aspects of the reconstruction procedure and further numerical examples are given in the author's thesis [20], of which the results presented in this paper are part.

2 The inverse problem

As input data for the inverse Dirichlet problem (IDP) treated in this paper, we are given real numbers $\nu_1 < \nu_2 < \dots < \nu_n$ and symmetric *basis functions*

$$\hat{q}(x), q_j(x), \quad j = 1, 2, \dots, n.$$

We seek a potential

$$q(x) = q(x; a) := \hat{q}(x) + \sum_{j=1}^n a_j q_j(x), \quad (2)$$

where $a = (a_j) \in \mathbb{R}^n$, so that

$$\lambda_i(q(x; a)) = \nu_i \quad \text{for } i = 1, 2, \dots, n, \quad (3)$$

that is, the lowest n eigenvalues of $q(x; a)$ correspond to the numbers ν_i .

Thus, (IDP) has become the finite-dimensional problem of determining $a \in \mathbb{R}^n$ so that the system of n nonlinear equations defined by (3) holds. Setting

$$f(a) = (f_i(a)) := (\lambda_i(q(x; a)) - \nu_i), \quad i = 1, 2, \dots, n, \quad (4)$$

Newton's method applied to $f(a) = 0$ defines a reconstruction procedure for (IDP), for

$$f(a) = 0 \Leftrightarrow q(x; a) \text{ solves (IDP).}$$

Applying Newton's method to $f(a) = 0$, we compute a sequence of iterated vectors

$$a^{(k+1)} := a^{(k)} - \left(\frac{\partial f_i}{\partial a_j}(a^{(k)}) \right)^{-1} f(a^{(k)}), \quad k = 0, 1, \dots, \quad (5)$$

and corresponding potentials

$$q^{(k)}(x) := q(x; a^{(k)}) = \hat{q}(x) + \sum_{j=1}^n a_j^{(k)} q_j(x), \quad k = 0, 1, \dots,$$

where the latter may be interpreted as approximate solutions of (IDP). The partial derivatives in the Jacobian of f are

$$\frac{\partial f_i}{\partial a_j}(a) = \int_0^\pi q_j(x) g_i^2(x; a) dx,$$

which follows from [23], §2, Theorem 3. Here, $g_i(x; a)$ denotes the L^2 -normalized i -th eigenfunction of $q(x; a)$ with $g_i'(0; a) > 0$.

We summarize this iteration in Algorithm 1:

Algorithm 1 Reconstruction procedure for (IDP) Newton's method
<p>1. Choose $a^{(0)} \in \mathbb{R}^n$.</p> <p>2. For $k = 0, 1, \dots$:</p> <p style="margin-left: 20px;">(i) For $i = 1, 2, \dots, n$:</p> <p style="margin-left: 40px;">(a) Compute $f_i(a^{(k)}) = \lambda_i(q^{(k)}) - \nu_i$.</p> <p style="margin-left: 40px;">(b) Compute $g_i(x; a^{(k)})$.</p> <p style="margin-left: 20px;">(ii) Compute the Jacobian</p> $\left(\frac{\partial f_i}{\partial a_j}(a^{(k)}) \right) = \left(\int_0^\pi g_i^2(x; a^{(k)}) q_j(x) dx \right), \quad i, j = 1, 2, \dots, n.$ <p style="margin-left: 20px;">(iii) Perform the Newton step</p> $a^{(k+1)} := a^{(k)} - \left(\frac{\partial f_i}{\partial a_j}(a^{(k)}) \right)^{-1} f(a^{(k)}).$

If an approximate solution \tilde{q} to the inverse problem is known, then \tilde{q} can be used to choose the starting vector $a^{(0)}$ in algorithm 1 and the basis functions for the reconstruction. In [20], p. 49, the following theorem has been proved:

Theorem 1 Consider the inverse Dirichlet problem with given numbers $\{\nu_i\}_{i=1}^n$. Suppose we are given an approximate potential $\tilde{q}(x)$ with eigenvalues $\{\tilde{\lambda}_i\}_{i=1}^n$. Now choose the basis functions

$$\begin{aligned}\hat{q}(x) &:= \tilde{q}(x), \\ q_j(x) &:= -2\frac{d}{dx}v_j, \quad j = 1, 2, \dots, n,\end{aligned}$$

where $v_j(x) = y_{1j}(x)y_{2j}(x)$ and y_{1j}, y_{2j} are the solutions of the initial value problems

$$\begin{aligned}-y''_{ij} + \tilde{q}(x)y_{ij} &= \tilde{\lambda}_j y_{ij}, \quad i = 1, 2 \\ y_{1j}(0) &= 1, \quad y'_{1j}(0) = 0 \\ y_{2j}(0) &= 0, \quad y'_{2j}(0) = 1.\end{aligned}\tag{6}$$

Let

$$\begin{aligned}\delta &:= \sum_{j=1}^n \|q_j\|, \\ \kappa &> \frac{1}{16\pi\delta^2 \max_{j=1}^n \|y_{1j}\| \|y_{2j}\|},\end{aligned}$$

and

$$\gamma := 16\pi\delta^2 \max_{j=1}^n \|y_{1j}\| \|y_{2j}\| e^{8\pi\kappa\delta \|y_{1j}\| \|y_{2j}\|}.$$

If

$$\max_{j=1}^n |\nu_j - \tilde{\lambda}_j| < \frac{1}{2\gamma},\tag{7}$$

then the iterated potentials of Algorithm 1 with starting vector $a^{(0)} = 0$ converge to a solution $q^*(x) = q(x; a^*)$ of the inverse Dirichlet problem, and the estimate

$$\|a^* - a^{(1)}\| \leq 2\gamma \|a^{(1)}\|^2$$

holds.

$\|\cdot\|$ denotes the infinity norm in $C[0, \pi]$ and in \mathbb{R}^n , respectively. The proof of the theorem makes use of the Newton-Kantorovich theorem ([22], p. 155). For $\hat{q}(x) \equiv c$, $c \in \mathbb{R}$, we obtain $q_1(x) = 1$, $q_{j+1}(x) = \cos(2jx)$, $j = 1, \dots, n-1$, which corresponds to a finite trigonometric expansion of $q(x)$.

As a consequence of this theorem, the reconstruction procedure is relieved from any *a priori*-restriction on the infinity norm of the unknown potential $q(x)$. The choice of $q_j(x)$ is motivated by results from [23]. For $\tilde{q}(x) \not\equiv c$, the finite trigonometric expansion of $q - \tilde{q}$ is replaced by linear combinations of the functions q_j . Unfortunately, the practical applicability of Theorem 1 is reduced considerably by inequality (7), which makes great demands on the quality of the approximate solution \tilde{q} .

3 Computation of eigenvalues and eigenfunctions

In each iteration step 2(i) of Algorithm 1, the lowest n eigenvalues of $q^{(k)}(x)$ and their corresponding eigenfunctions have to be computed. We do this by applying the shooting method to the initial value problem

$$\begin{aligned} -u'' + q(x)u &= \lambda u, & x \in [0, \pi] \\ u(0) &= 0, & u'(0) = 1. \end{aligned} \tag{8}$$

For a fixed potential $q(x)$, we denote the solution of (8) by $u(x, \lambda)$. If $q(x)$ is regarded as a variable, too, we use the notation $u(x; q, \lambda)$.

To compute eigenvalue bounds, we make use of the well-known fact that the number of zeroes of $u(x, \lambda)$ in the interval $[0, \pi]$ is an increasing function of λ , and that the i -th eigenfunction of the Dirichlet problem has exactly $i - 1$ simple zeroes in $(0, \pi)$. These properties hold for a large class of Sturm-Liouville problems, see e.g. [9].

Counting the zeroes of $u(x, \lambda)$ in $(0, \pi)$ for some $\lambda \in \mathbb{R}$, we get bounds for the eigenvalues of $q(x)$. By iterating with respect to λ , these bounds can be made arbitrarily sharp (see [19], [20] for numerical examples).

Once λ_i is known, the i -th eigenfunction $u_i(x)$ of $q(x)$, normalized so that $u'_i(0) = 1$, can be computed by solving the initial value problem (8), with the exact eigenvalue λ_i inserted for λ . Finally, the L^2 -normalized eigenfunction $g_i(x)$ is obtained by evaluating $\int_0^\pi u_i^2(x) dx$.

4 Inclusion of a solution

We have already remarked that the requirements of Theorem 1 are not likely to be fulfilled in practical applications. Therefore, we use interval Newton's method applied to $f(a) = 0$ (where f is defined by (4)) to compute enclosures of a solution of the inverse Dirichlet problem. Before we describe the inclusion procedure, we introduce some notation. For a detailed introduction to interval computations, see [1].

Real bounded and closed intervals are denoted by $[a] = [\underline{a}, \bar{a}]$, $[b] = [\underline{b}, \bar{b}]$, etc. The same notation is used for interval vectors, e.g. $[a] = ([a_i])$. The space of m -dimensional interval vectors is denoted by $I\mathbb{R}^m$. Real (m, m) -matrices are denoted by $A = (a_{ij})$, the corresponding interval matrices by $[A] = ([a_{ij}])$.

By applying Gaussian elimination algorithm to an (m, m) -interval matrix $[A]$ and an interval vector $[b]$ with m components, we compute an interval vector $[x]$, so that

$$\{ x = A^{-1}b \mid A \in [A], b \in [b] \} \subseteq [x]$$

holds ([1], §15). We denote this vector $[x]$ by IGA($[A], [b]$).

A pair of continuous functions \underline{w} , \bar{w} , satisfying $\underline{w}(x) \leq \bar{w}(x)$ in $D \subseteq \mathbb{R}$, define an *interval function*

$$\begin{aligned} [w](x) &:= [\underline{w}(x), \bar{w}(x)] \\ &:= \{ w(x) \in C^0(D) \mid \underline{w}(x) \leq w(x) \leq \bar{w}(x) \text{ for all } x \in D \}. \end{aligned}$$

We denote by $q(x; [a])$ a set of linear combinations of the basis functions in the reconstruction procedure, namely

$$\begin{aligned} q(x; [a]) &:= \hat{q}(x) + \sum_{i=1}^n [a_i] q_i(x) \\ &:= \{ \hat{q}(x) + \sum_{i=1}^n a_i q_i(x) \mid a_i \in [a_i] \}. \end{aligned} \tag{9}$$

It is most important for the implementation of the inclusion procedure that the function set $q(x; [a])$ is amenable to symbolic calculations such as symbolic integration or differentiation. E.g., if the basis functions are differentiable, then symbolic differentiation (that is, treating interval coefficients like real constants) of (9) is possible and yields enclosures of the derivatives of all $q(x) \in q(x; [a])$:

$$\{ q'(x) \mid q(x) \in q(x; [a]) \} = \hat{q}'(x) + \sum_{i=1}^n [a_i] q_i'(x).$$

The interval function $g_i(x; [a])$ denotes the result of an interval-arithmetic computation of eigenfunctions, so that

$$\{ g_i(x; a) \mid a \in [a] \} \subseteq g_i(x; [a]).$$

Similarly, the interval-arithmetic evaluation of the derivative of f on $[a]$ is given by the interval matrix $\frac{\partial f_i}{\partial a_j}([a])$, where

$$\left\{ \left(\frac{\partial f_i}{\partial a_j}(a) \right) \mid a \in [a] \right\} \subseteq \left(\frac{\partial f_i}{\partial a_j}([a]) \right).$$

The interval Newton operator corresponding to (5) is defined by

$$\text{IN}([a]) := m([a]) - \text{IGA} \left(\frac{\partial f_i}{\partial a_j}([a]), f(m([a])) \right),$$

where $m : I\mathbb{R}^n \rightarrow \mathbb{R}^n$, $m([a]) \in [a]$ denotes a selection procedure for a real vector $m([a])$ from the interval vector $[a]$. Usually, $m([a])$ is taken to be the midpoint of each component of $[a]$. The interval Newton operator has the property (see [2]) that if

$$\text{IN}([a]) \subseteq [a], \tag{10}$$

then $\text{IN}([a])$ encloses a unique zero of f .

The interval version of Algorithm 1 is given by the following reconstruction procedure:

Algorithm 2 Reconstruction procedure for (IDP)
Interval Newton's method

1. Choose $[a]^{(0)} \in IR^n$.

2. For $k = 0, 1, \dots$:

(i) For $i = 1, 2, \dots, n$:

(a) Compute $f_i(m^{(k)}) = \lambda_i(q_m^{(k)}) - \nu_i$,

(b) Compute $g_i(x; [a]^{(k)})$,

where

$$m^{(k)} := m([a]^{(k)}),$$

$$q_m^{(k)}(x) := q(x; m^{(k)}) := \hat{q}(x) + \sum_{j=1}^n m_j^{(k)} q_j(x).$$

(ii) Compute the Jacobian

$$\left(\frac{\partial f_i}{\partial a_j}([a]^{(k)}) \right) = \left(\int_0^\pi g_i^2(x; [a]^{(k)}) q_j(x) dx \right),$$

$i, j = 1, 2, \dots, n.$

(iii) Perform the interval Newton step

$$\text{IN}([a]^{(k)}) := m^{(k)} - \text{IGA} \left(\left(\frac{\partial f_i}{\partial a_j}([a]^{(k)}) \right), f(m^{(k)}) \right),$$

$$[a]^{(k+1)} := \text{IN}([a]^{(k)}) \cap [a]^{(k)}.$$

From the inclusion property (10) of the interval Newton operator, we deduce the following theorem:

Theorem 2 *Let $[a]^{(k)}$ be the sequence of interval vectors defined by Algorithm 2. Then if for one $k \in \mathbb{N}$*

$$\text{IN}([a]^{(k)}) \subseteq [a]^{(k)}, \tag{11}$$

then $[a]^{(k+1)}$ encloses exactly one solution a^ of $f(a) = 0$. The function set*

$$q(x; [a]^{(k+1)}) = \hat{q}(x) + \sum_{j=1}^n [a_j]^{(k+1)} q_j(x)$$

contains exactly one potential of the form (2), namely

$$q^*(x) := q(x; a^*) = \hat{q}(x) + \sum_{j=1}^n a_j^* q_j(x),$$

corresponding to the prescribed eigenvalues $\{\nu_i\}_{i=1}^n$.

Remark: In applications, inaccuracies of measurement usually prevent the determination of *exact* eigenvalues. Therefore, a rigid error estimation for the difference between

$q(x)$ and the reconstructed potential is desirable. Since Algorithm 2 also applies to *interval* eigenvalue data, we obtain safe error bounds (in the infinity norm) by using interval enclosures $[\nu_i]$ of eigenvalues instead of real numbers ν_i . Then $f(m^{(k)})$ becomes an interval vector, and in the interval Newton step, the interval vector $\text{IN}([a]^{(k)})$ must enclose all solutions x of the linear systems

$$A(x - m^{(k)}) = -y, \quad A \in \left(\frac{\partial f_i}{\partial a_j}([a]^{(k)}) \right), \quad y \in f(m^{(k)}). \quad (12)$$

For this purpose, one of the methods described in [21] can be applied instead of interval Gaussian elimination.

5 Eigenvalue enclosures

In Section 3, eigenvalue *approximations* were computed by the shooting method. In this section, we compute guaranteed eigenvalue *enclosures* by a modification of the shooting method. With Lohner's enclosure method for the solutions of ordinary initial value problems implemented in his PASCAL-XSC program called AWA ([14], [15], [16]), we compute an interval function $[u](x)$ that contains the true solution $u(x)$ of (8).

Again, we compute eigenvalue bounds by counting zeroes. In order to count the correct number of zeroes, we have to guarantee that whenever the interval function $[u](x)$ crosses the x -axis, $u(x)$ has *exactly one* zero there. To guarantee this, we compute an enclosure $[u'](x)$ of $u'(x)$ as well, and verify that $0 \in [u](x)$ and $0 \notin [u'](x)$ hold simultaneously for $x \in [0, \pi]$. As all zeroes of $u(x)$ are simple, the correct number of zeroes can be computed if the function enclosures of the solutions of (8) are sharp enough.

Replacing $q(x; a)$ in (8) by $[q](x) := q(x; [a])$ and applying AWA to the resulting initial value problem, we get simultaneous enclosures of the eigenvalues of all potentials $q(x; a) \in [q](x)$, due to the inclusion monotonicity of the interval operations. To make AWA applicable, $[q](x)$ must be interpreted as a function set in the sense of (9). However, numerous calculations have shown that the eigenvalue bounds computed using this approach are not very tight if the *diameter*

$$d([q]) := \max_{x \in [0, \pi]} (\bar{q}(x) - \underline{q}(x))$$

of $[q](x)$ is large. In this case, we make use of a monotonicity argument.

With two eigenvalue bounds $\lambda_i(q_{mid})$ and $\bar{\lambda}_i(q_{mid})$ of the *midpoint function*

$$q_{mid}(x) := \frac{1}{2} (\underline{q}(x) + \bar{q}(x))$$

of $[q](x)$, and the estimate

$$\|q(x) - q_{mid}(x)\|_\infty \leq \frac{1}{2} d([q]),$$

we obtain the bounds

$$\lambda_i(q_{mid}) - \frac{1}{2}d([q]) \leq \lambda_i(q) \leq \bar{\lambda}_i(q_{mid}) + \frac{1}{2}d([q]) \quad (13)$$

for the eigenvalues of any $q(x) \in [q](x)$.

In our numerical examples which we will present in Section 8, we define the selection procedure m in the interval Newton step of Algorithm 2 to choose the midpoint of the interval vector $[a]^{(k)}$. In this case, eigenvalue bounds of $q_{mid}^{(k)}(x)$ are already necessary to perform the iteration. Therefore, to enclose the eigenvalues of $[q]^{(k)}(x) := q(x; [a]^{(k)})$ with the aid of (13), we merely have to compute or estimate the diameter of $[q]^{(k)}(x)$, so that with this method, sharp enclosures of eigenvalues of all potentials $q(x) \in [q]^{(k)}(x)$ can be obtained with modest amount of work. These eigenvalue enclosures will be used to enclose the eigenfunctions $g_i(x)$.

6 Eigenfunction enclosures

If we allow an interval $[\lambda]$ instead of the real parameter λ in the application of AWA to (8), we compute an interval function $u(x, [\lambda])$ satisfying

$$u(x, \lambda) \in u(x, [\lambda]) \quad \text{for all } x \in [0, \pi] \text{ and all } \lambda \in [\lambda].$$

This property is used to obtain eigenfunction enclosures for $q(x)$ in two steps.

First, we compute an enclosure $[\lambda_i]$ of the i -th eigenvalue λ_i of $q(x)$. Then we apply AWA to (8) with $[\lambda] = [\lambda_i]$. Because

$$u_i(x) = u(x, \lambda_i) \in u(x, [\lambda_i]) \quad \text{for all } x \in [0, \pi],$$

the interval function $u(x, [\lambda_i])$ encloses the i -th eigenfunction $u_i(x)$ of $q(x)$.

Finally, we insert interval data for both $q(x)$ and λ , apply AWA to (8), and compute an interval function $[u](x) := u(x; [q], [\lambda])$ which satisfies

$$u(x; q, \lambda) \in u(x; [q], [\lambda]) \quad \text{for all } x \in [0, \pi], \text{ all } q(x) \in [q](x) \text{ and all } \lambda \in [\lambda].$$

To obtain simultaneous enclosures of the normalized eigenfunctions of all $q(x) \in [q](x)$, we compute an interval $[\lambda_i] \supseteq \{\lambda_i(q) \mid q(x) \in [q](x)\}$ by the method described in the previous section. After that, we apply AWA to (8) to compute the interval function $u(x; [q], [\lambda_i])$ containing the i -th eigenfunctions $u_i(x)$ of all $q(x) \in [q](x)$.

To proceed, we have to give a precise description of the structure of $u(x; [q], [\lambda_i])$. Applying AWA, the interval $[0, \pi]$ is divided into equidistant subintervals $[x_l, x_{l+1}]$, $l = 0, 1, \dots, l_{max} - 1$. In each subinterval $[x_l, x_{l+1}]$, we compute intervals $[c_k]$, $k = 0, 1, \dots, r$, that enclose the Taylor coefficients up to order $r - 1$ and the corresponding remainder term of all $u_i(x) = u(x; q, \lambda_i(q))$ with $q(x) \in [q](x)$. Hence, for all $q(x) \in [q](x)$,

$$u_i(x) \in u(x; [q], [\lambda_i]) := \sum_{k=0}^r [c_k](x - x_l)^k, \quad x \in [x_l, x_{l+1}]. \quad (14)$$

This representation allows us to compute enclosures of squares of eigenfunctions by squaring $u(x; [q], [\lambda_i])$ in each subinterval $[x_l, x_{l+1}] \subset [0, \pi]$. We get an enclosure of $u_i^2(x)$ in the form

$$u_i^2(x) \in \sum_{k=0}^{2r} [d_k](x - x_l)^k, \quad x \in [x_l, x_{l+1}]. \quad (15)$$

Since $(x - x_l)^k$ does not change sign in $[x_l, x_{l+1}]$, when integrating (15) we may write the interval coefficients $[d_k]$ before the integral ([13], p. 29) to obtain

$$\int_{x_l}^{x_{l+1}} u_i^2(x) dx \in \sum_{k=0}^{2r} [d_k] \int_{x_l}^{x_{l+1}} (x - x_l)^k dx.$$

Summation over all subintervals of $[0, \pi]$ results in an interval $[z_i]$, which contains $\|u_i^2\|_2^2$ for all $q(x) \in [q](x)$. Division

$$[g_i](x) := \frac{[u_i](x)}{\sqrt{[z_i]}}$$

yields an enclosure of the L^2 -normalized eigenfunctions $g_i(x)$ of all $q(x) \in [q](x)$ of the form (14). We used this interval function to enclose the Jacobian in Algorithm 2 in an interval matrix.

7 Enclosures of the partial derivatives

The final step to enclose the elements of the Jacobian is to evaluate the integrals

$$\int_0^\pi [g_i]^2(x) q_j(x) dx. \quad (16)$$

We compute enclosures of the form (14) for all basis functions $q_j(x)$, using the same breakpoints as for the $[g_i](x)$. After that, the integrals (16) have been calculated by symbolic multiplication of these interval functions, followed by symbolic integration as in the previous section.

We summarize the necessary steps to enclose the Jacobian $\left(\frac{\partial f_i}{\partial a_j}([a])\right)$:

For $i = 1, 2, \dots, n$:

1. Compute an enclosure $[\lambda_i]$ of the i -th eigenvalues of all $q(x) \in [q](x) := q(x; [a])$.
2. For all $q(x) \in [q](x)$, $\lambda_i \in [\lambda_i]$, enclose the solutions of

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

in the interval function $[u_i](x)$.

3. Compute an enclosure $[z_i]$ of $\int_0^\pi u_i^2 dx$ for all $u_i(x) \in [u_i](x)$.

$$\text{Let } [g_i](x) := \frac{[u_i](x)}{\sqrt{[z_i]}}.$$

For $j = 1, 2, \dots, n$:

$$\text{Let } \frac{\partial f_i}{\partial a_j}([a]) := \int_0^\pi [g_i]^2(x) q_j(x) dx.$$

Evaluate the integral by symbolic calculations as described in Section 6.

8 Numerical results

The numerical performance of the reconstruction procedure in this paper is much more expensive than the algorithms for approximate solutions mentioned in the introduction. The computation of enclosures of the function value of f and of the Jacobian in Algorithm 2 requires solving $2n$ eigenvalue problems (by the method described in Section 5, this can be reduced to the computation of only n eigenvalues). To obtain eigenvalue bounds with the shooting method requires solving several interval-valued initial value problems for *each* of these eigenvalues. An additional n initial value problems have to be solved to compute the eigenfunctions needed in the Jacobian. The computation of the Jacobian also requires the evaluation of n^2 integrals. The large amount of work is justified in many applications by the possibility to validate the existence of a solution numerically on the computer and to investigate the sensitivity of the reconstructed potential to variations in the prescribed eigenvalues by permitting interval data in the reconstruction.

On the other hand, *approximate* solutions can be obtained rather cheaply by approximately solving the eigenvalue problems with the Rayleigh–Ritz method. As the i -th eigenfunction of the Sturm-Liouville equation resembles $\sin(ix)$, the sine functions supply excellent basis functions for the Rayleigh–Ritz method, thus reducing the eigenvalue problem to the computation of *matrix* eigenvalues and eigenvectors.

In our numerical examples, we used the Rayleigh–Ritz method as the initial step of the reconstruction procedure to compute an approximate solution that was further improved by two or three steps of Algorithm 1 (performed in real machine arithmetic). An assumed enclosure $[q]^{(0)}(x)$ of a solution of (IDP) was obtained using criteria from [3] for the determination of a starting interval for interval Newton’s method from iterates of real Newton iteration. With the implementation of Algorithm 2 on a computer, the existence and inclusion of such a solution was finally proved. In all examples, only one step of Algorithm 2 was needed for that proof. To make the numerical existence proof rigorous, all rounding errors were enclosed in the computation.

To demonstrate that the use of interval arithmetic can produce tight enclosures of the solutions, we used function sets that include the desired potentials in the reconstruction procedure. We present two examples. In one example, a finite trigonometric

expansion of q is used (cf. the remark in Section 2). In the other example, symmetric cubic splines (as an example of a function set suitable for the approximation of smooth functions) are used. In both examples, potentials with extremely large infinity norm are reconstructed ($\|q\|_\infty$ is about 20–100 times larger than in the examples presented in [5], [17], [18], [24], [25]).

Of course, the input data of the reconstruction problem usually consists of n real numbers not exactly representable in finite arithmetic. With our method, intervals accounting for roundoff errors or errors of measurements can be used instead of the exact values. With these, distinct inverse problems can be solved at the same time, and a sensitivity analysis of the inverse problem is also accomplished.

Hence, as input data for the reconstruction, in both examples we compare machine representable approximations of the eigenvalues with interval enclosures of the eigenvalues of different accuracy. Of course, when the eigenvalues are prescribed to 16 decimal digits and are not infinitely exact, with sufficiently precise arithmetic we could compute an enclosure of the solution to the 16 digits inverse problem that does not enclose $q(x)$.

The examples presented here were computed using the 16 decimal digit real and interval arithmetic of PASCAL-XSC (guaranteeing identical results on any machine). On an HP personal computer with an Intel 486-processor (66MHz), about fifteen to twenty minutes were needed to perform the calculations of one reconstruction. Most of the computation time was consumed by the enclosure step. The solutions of the initial value problems (8) were enclosed with a variant of Lohner's program AWA, adapted to the rather simple structure of the differential equation. To enclose the solutions of the linear systems in the interval Newton step, the PASCAL-XSC problem solving routine LSS was used instead of interval Gaussian elimination.

The complete code is available on request to the author's e-mail address.

Example 1: Reconstruction of $q(x) = 100 \left(\frac{2}{\pi}x - 1 \right)^2$ from four eigenvalues

Function set for $q(x)$: Symmetric cubic spline with 8 knots, $x_i = i\pi/7$, $i = 0, 1, \dots, 7$.

$$q_j(x_{i-1}) = q_j(x_{8-i}) = \delta_{ij}, \quad i, j = 1, 2, 3, 4.$$

Initial guess: $q^{(0)}(x) = 0$.

a) Prescribed eigenvalues: 16 decimal digit approximations:

$$\nu_1 = 6.366\ 206\ 010\ 508\ 312, \quad \nu_2 = 19.098\ 834\ 811\ 432\ 28,$$

$$\nu_3 = 31.834\ 245\ 487\ 078\ 10, \quad \nu_4 = 44.590\ 112\ 710\ 479\ 30.$$

Enclosures in the breakpoints:

$$[q](0) = \frac{100.000}{99.999} \frac{000}{999} \frac{000}{999} \frac{149}{851} \frac{3}{92}, \quad [q](\pi/7) = 51.020\ 408\ 163\ 2_{55}^{75} \frac{49}{22},$$

$$[q](2\pi/7) = 18.367\ 346\ 938\ 77_4^6 \frac{28}{75}, \quad [q](3\pi/7) = 2.040\ 816\ 326\ 530 \frac{814}{413}.$$

b) Prescribed eigenvalues: tight interval enclosures:

$$\begin{aligned}\nu_1 &= 6.366\ 206\ 010\ 508\ \frac{366}{258}, & \nu_2 &= 19.098\ 834\ 811\ 432\ \frac{39}{16}, \\ \nu_3 &= 31.834\ 245\ 487\ 07\ \frac{8}{7}\ \frac{23}{96}, & \nu_4 &= 44.590\ 112\ 710\ 479\ \frac{47}{13}.\end{aligned}$$

Enclosures in the breakpoints:

$$\begin{aligned}[q](0) &= \frac{100.000}{99.999}\ \frac{000}{999}\ \frac{000}{999}\ \frac{718}{281}\ \frac{8}{88}, & [q](\pi/7) &= 51.020\ 408\ 163\ \frac{312}{218}\ \frac{46}{22}, \\ [q](2\pi/7) &= 18.367\ 346\ 938\ 77\ \frac{9}{1}\ \frac{06}{96}, & [q](3\pi/7) &= 2.040\ 816\ 326\ \frac{531}{29}\ \frac{370}{854}.\end{aligned}$$

c) Prescribed eigenvalues: 10 dezimal digit interval enclosures:

$$\begin{aligned}\nu_1 &= 6.366\ 206\ 01_0^1, & \nu_2 &= 19.098\ 834\ 8_1^2, \\ \nu_3 &= 31.834\ 245\ 4_8^9, & \nu_4 &= 44.590\ 112\ 7_1^2.\end{aligned}$$

Enclosures in the breakpoints:

$$\begin{aligned}[q](0) &= \frac{100.000}{99.999}\ \frac{005}{998}\ \frac{455}{186}\ \frac{594}{155}\ \frac{6}{99}, & [q](\pi/7) &= 51.020\ 408\ \frac{518}{052}\ \frac{437}{080}\ \frac{80}{21}, \\ [q](2\pi/7) &= 18.367\ 346\ 9\ \frac{54}{15}\ \frac{403}{603}\ \frac{94}{61}, & [q](3\pi/7) &= 2.040\ 816\ \frac{333}{19}\ \frac{700}{540}\ \frac{984}{180}.\end{aligned}$$

Example 2: Reconstruction of $q(x) = 100 \cos(10x)$ from six eigenvalues

Function set for $q(x)$: $q(x; a) = a_0 + \sum_{j=1}^5 a_j \cos(2jx)$.

Initial guess: $q^{(0)}(x) = 99 \cos(10x)$.

a) Prescribed eigenvalues: 16 decimal digit approximations:

$$\begin{aligned}\nu_1 &= -37.575\ 466\ 563\ 677\ 14, & \nu_2 &= -36.840\ 425\ 617\ 896\ 98, \\ \nu_3 &= -35.890\ 355\ 745\ 793\ 39, & \nu_4 &= -35.084\ 400\ 836\ 106\ 08, \\ \nu_5 &= -34.766\ 912\ 530\ 639\ 00, & \nu_6 &= 61.476\ 539\ 932\ 499\ 41.\end{aligned}$$

Enclosure: $[q](x) = [-2.475 \cdot 10^{-9}, 2.454 \cdot 10^{-9}]$

$$\begin{aligned}&+ [-6.277 \cdot 10^{-9}, 6.224 \cdot 10^{-9}] \cos(2x) + [-6.229 \cdot 10^{-9}, 6.175 \cdot 10^{-9}] \cos(4x) \\ &+ [-6.811 \cdot 10^{-9}, 6.754 \cdot 10^{-9}] \cos(6x) + [-8.063 \cdot 10^{-9}, 7.998 \cdot 10^{-9}] \cos(8x) \\ &+ (100 + [-3.624 \cdot 10^{-9}, 3.595 \cdot 10^{-9}]) \cos(10x).\end{aligned}$$

b) Prescribed eigenvalues: tight interval enclosures:

$$\begin{aligned}\nu_1 &= -37.575\ 466\ 563\ 6\ \frac{69}{84}\ \frac{40}{88}, & \nu_2 &= -36.840\ 425\ 617\ \frac{870}{923}\ \frac{27}{68}, \\ \nu_3 &= -35.890\ 355\ 745\ \frac{696}{890}\ \frac{32}{44}, & \nu_4 &= -35.084\ 400\ 836\ \frac{022}{189}\ \frac{44}{72}, \\ \nu_5 &= -34.766\ 912\ 530\ 6\ \frac{01}{76}\ \frac{78}{22}, & \nu_6 &= 61.476\ 539\ 932\ \frac{512}{486}\ \frac{59}{21}.\end{aligned}$$

Enclosure: $[q](x) = [-4.917 \cdot 10^{-9}, 4.909 \cdot 10^{-9}]$

$$\begin{aligned}&+ [-1.247 \cdot 10^{-8}, 1.245 \cdot 10^{-8}] \cos(2x) + [-1.240 \cdot 10^{-8}, 1.241 \cdot 10^{-8}] \cos(4x) \\ &+ [-1.356 \cdot 10^{-8}, 1.357 \cdot 10^{-8}] \cos(6x) + [-1.602 \cdot 10^{-8}, 1.600 \cdot 10^{-8}] \cos(8x) \\ &+ (100 + [-7.200 \cdot 10^{-9}, 7.188 \cdot 10^{-9}]) \cos(10x).\end{aligned}$$

c) Prescribed eigenvalues: 10 decimal digit interval enclosures:

$$\begin{aligned}\nu_1 &= -37.575\,466\,5_7^6, & \nu_2 &= -36.840\,425\,6_2^1, \\ \nu_3 &= -35.890\,355\,7_5^4, & \nu_4 &= -35.084\,400\,8_4^3, \\ \nu_5 &= -34.766\,912\,5_4^3, & \nu_6 &= 61.476\,539\,9_3^4.\end{aligned}$$

$$\begin{aligned}\text{Enclosure: } [q](x) &= [-4.284 \cdot 10^{-7}, 1.934 \cdot 10^{-7}] \\ &+ [-1.085 \cdot 10^{-6}, 4.778 \cdot 10^{-7}] \cos(2x) + [-1.058 \cdot 10^{-6}, 3.806 \cdot 10^{-7}] \cos(4x) \\ &+ [-1.140 \cdot 10^{-6}, 4.124 \cdot 10^{-7}] \cos(6x) + [-1.380 \cdot 10^{-6}, 6.022 \cdot 10^{-7}] \cos(8x) \\ &+ (100 + [-6.231 \cdot 10^{-7}, 2.865 \cdot 10^{-7}]) \cos(10x).\end{aligned}$$

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