Journal of Universal Computer Science, vol. 4, no. 2 (1998), 178-192
submitted: 25/9/97, accepted: 1/11/97, appeared: 28/2/98

Enclosing Solutions of an inverse Sturm-Liouville problem for an impedance

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Abstract: This paper is concerned with the reconstruction of an unknown impedance $p(x)$ 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 $[p](x)$ is constructed that encloses an impedance $p(x)$ corresponding to the prescribed eigenvalues. To make this numerical existence proof rigorous, all discretization and roundoff errors have to be taken into account in the computation.

Key Words: Inverse Sturm-Liouville problem, Enclosure methods, Validated numerics

1 Introduction

Consider the impedance case of the Sturm-Liouville problem with Dirichlet boundary conditions:

$$\begin{aligned} (p(x)u')' \; + \; \lambda p(x)u &= 0 \\ u(0) \; = \; u(\pi) &= 0, \end{aligned} \tag{1}$$

where the impedance $p(x)$ is assumed to be continuously differentiable in $[0,\pi]$, symmetric about $\frac{\pi}{2}$ (that is, $p(x) = p(\pi - x)$ holds for all $x \in [0,\pi]$) and positive, with $p(0) = 1$. Apart from other applications, equation (1) describes longitudinal vibrations of a thin straight rod [7]. Here, $p(x)$ represents the cross–sectional area of the rod.

The established theory extends well beyond the above regularity assumptions. However, to obtain good numerical results, derivatives of even higher order are required so that we are not concerned with weak solutions of (1) of any kind.

A real number λ is called an eigenvalue of (1) if there is a nontrivial solution $u(x)$ of the boundary value problem (1). $u(x)$ is then 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 distinct positive real numbers that tend to infinity. In the above setting, the eigenvalues can be interpreted as functionals of the impedance $p(x)$, denoted by $\lambda_i(p)$, $i \in I\!N$, in increasing order: $0 < \lambda_1(p) < \lambda_2(p) < \dots$.

The impedance problem (1) is closely linked with the following potential problem (3). If $p(x)$ is smooth enough, let

$$q(x) = \frac{\sqrt{p(x)}''}{\sqrt{p(x)}}, \quad y(x) = \sqrt{p(x)}u(x) \tag{2}$$

to obtain

$$\begin{aligned} -y'' \ + \ q(x)y &= \lambda y \\ y(0) \ = \ y(\pi) &= 0. \end{aligned} \tag{3}$$

Due to its physical meaning, $q(x)$ is called a potential function.

As is expected from the transformation (2), the eigenvalue problems (1) and (3) have many common properties, e.g. similar asymptotic expansions of their eigenvalues or similar distributions of the zeros of corresponding eigenfunctions. In fact, most of the theory developed for either of (1) and (3) carries over to the other problem. It is mainly in the existing computational algorithms that one can tell (1) from (3).

The opposite of the computation of eigenvalues and eigenfunctions of (1) for a given impedance $p(x)$ (or of (3) for a given potential $q(x)$), the inverse problem is concerned with the reconstruction of $p(x)$ in (1) (or $q(x)$ in (3)) from spectral data. The inverse formulation was first considered for the potential problem, and until today, in most papers on the reconstruction of Sturm–Liouville operators the potential case is investigated. This is even more true for the development of numerical algorithms.

In his fundamental paper [5], Borg proved in 1946 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 (3). The first numerical scheme for the potential case was originated by Gel'fand and Levitan [6] in 1951. Since then, a large variety of reconstruction procedures have been suggested (cf. [3, 4, 7, 10, 18, 19, 27]; further references are given in [7, 18]). The reconstruction of an impedance without reconstructing a potential first and then using (2) to procure the impedance, has only recently attracted more attention (cf. [13, 26]).

In a neighborhood of $q(x) = 0$, local existence of a solution of the inverse problem with finitely many given eigenvalues can be proved for finite Fourier expansions of q. A popular approach is to assume a finite trigonometric expansion of q and recover the Fourier coefficients from the given eigenvalues ([9, 18]). The same technique was used in [13] in a neighborhood of $p(x) = 1$ in the impedance case.

In [21, 22], a numerical scheme for the potential case with precise error bounds in the infinity norm was given for the first time. In this paper, the same task is accomplished for the impedance case. All necessary computations of the reconstruction procedure and of the error bounds can be carried out on a computer, if discretization and roundoff errors are enclosed.

The paper is structured as follows: In Section 2, the reconstruction of $p(x)$ from given eigenvalues is transformed into a system of nonlinear equations, that is solved with Newton's method. In each Newton step, the direct problem has to be solved. Hence, the computation of eigenvalues and eigenfunctions of (1) is discussed in Section 3. Applying interval Newton's method to the nonlinear system, in Section 4 the existence and local uniqueness of a solution of the system is validated. This solution is enclosed in an interval vector, with which we construct an interval function $[p](x)$ that encloses a solution $p(x)$ of the inverse impedance problem. In sections 5 and 6, algorithms for the validated solution of the direct problem are presented. In the last section, the practical applicability of the method is demonstrated with numerical examples.

2 The inverse problem

The input data for the inverse impedance problem treated in this paper are real numbers $\nu_1 < \nu_2 < \ldots < \nu_n$, an approximate impedance $\widehat{p}(x)$ with eigenvalues μ_i ($\widehat{p}(x) = 1$ with $\mu_i = i^2$ may be used, if no better choice is at hand) and *basis functions*

$$p_j(x), \quad j = 1, 2, \ldots, n.$$

$\widehat{p}$ and the functions p_j are supposed to be differentiable, symmetric and to fulfill $\widehat{p}(0) = 1$, $\widehat{p}(x) > 0$ for $x \in [0, \pi]$ and $p_j(0) = 0$ for $j = 1, \ldots, n$.

We seek an impedance

$$p(x; a) := \widehat{p}(x) + \sum_{j=1}^{n} a_j \, p_j(x), \tag{4}$$

where $a = (a_j) \in I\!R^n$, so that

$$\lambda_i(p(x; a)) \;=\; \nu_i \quad \text{for} \;\; i = 1, 2, \ldots, n. \tag{5}$$

Thus, the inverse impedance problem has become the finite-dimensional problem of determining $a \in I\!R^n$ so that the system of n nonlinear equations defined by (5) holds. Setting

$$f(a) \;=\; (f_i(a)) \;:=\; (\lambda_i(p(x; a)) - \nu_i), \quad i = 1, 2, \ldots, n, \tag{6}$$

then by the definition of f,

$$f(a) \;=\; 0 \quad \Longleftrightarrow \quad p(x; a) \;\text{ fulfills }\; (5).$$

Following the analysis of Pöschel and Trubowitz in their comprehensive book [24] on the inverse potential problem, by straightforward (though tedious) calculations it can be shown that f is a continuously differentiable function with partial derivatives

$$\frac{\partial f_i}{\partial a_j}(a) \;=\; \int_0^\pi \left(g_i'^2(x; a) - \lambda_i g_i^2(x; a)\right) \, p_j(x) \, dx,$$

where $g_i(x, a)$ denotes the i–th eigenfunction of (1) belonging to $p(x; a)$, normalized so that

$$\int_0^\pi p(x; a) g_i^2(x; a) \, dx \;=\; 1.$$

When function values of f and of the Jacobian are available, zeros of f can be computed with Newton's method. Due to the implicit function theorem and the Newton–Kantorovich theorem, the following theorem holds:

Theorem 1. *If the basis functions $p_j(x)$ are chosen so that the Jacobian of f at $a = 0$ is nonsingular, then there is a neighborhood of $\mu = (\mu_i) \in I\!R^n$ where (5) has a locally unique solution, where the Newton iterates starting with $a^{(0)} = 0$ converge to this solution and where the corresponding iterated impedance functions*

$$p^{(k)}(x) \;:=\; p(x; a^{(k)}) \;=\; \widehat{p}(x) + \sum_{j=1}^{n} a_j^{(k)} \, p_j(x), \quad k = 0, 1, \ldots,$$

are positive functions on $[0, \pi]$.

The reconstruction of $p(x;a)$ via Newton iteration applied to (6) is outlined in Algorithm 1:

Algorithm 1: Newton's Method

1. Let $a^{(0)} = 0$.
2. For $k = 0, 1, \ldots$:
   (i) Let $p^{(k)}(x) := \widehat{p}(x) + \sum_{j=1}^{n} a_j^{(k)}\, p_j(x)$.
   (ii) For $i = 1, 2, \ldots, n$:
      (a) Compute $f_i(a^{(k)}) = \lambda_i(p^{(k)}) - \nu_i$.
      (b) Compute $g_i(x; a^{(k)})$.
   (iii) Compute the Jacobian

$$\left(\frac{\partial f_i}{\partial a_j}(a^{(k)})\right) = \left(\int_0^\pi \left(g_i'^2(x;a) - \lambda_i g_i^2(x;a)\right)\, p_j(x)\, dx, \right)_{i,j=1,2,\ldots,n}$$

   (iv) Perform the Newton step

$$a^{(k+1)} := a^{(k)} - \left(\frac{\partial f_i}{\partial a_j}(a^{(k)})\right)^{-1} f(a^{(k)}).$$

To compute the function values of f and the elements of the Jacobian, in Step 2 (ii) of Algorithm 1, the direct problem has to be solved. More precisely, the lowest n eigenvalues of $p^{(k)}(x)$ and their corresponding eigenfunctions have to be determined. Suitable algorithms are presented in the next section.

3 Computation of eigenvalues and eigenfunctions

The direct problem can be solved by applying the shooting method to the initial value problem

$$\begin{aligned} (p(x)u')' + \lambda p(x)u = 0, \quad x \in [0,\pi] \\ u(0) = 0, \quad u'(0) = 1. \end{aligned} \tag{7}$$

For a fixed impedance $p(x)$, we denote the solution of (7) by $u(x,\lambda)$. If $p(x)$ is regarded as a variable, too, the notation $u(x;p,\lambda)$ is used. We also let $\lambda_0 := -\infty$ in the following.

To compute eigenvalue bounds, we make use of the well-known fact that the number of zeros of $u(x,\lambda)$ in the interval $[0,\pi]$ is an increasing function of λ, and that the i-th eigenfunction of (1) has exactly $i-1$ simple zeros in $(0,\pi)$. These properties hold for a large class of Sturm-Liouville problems, see e.g. [8].

For some $\lambda \in \mathbb{R}$, compute $u(x,\lambda)$ and count the number $N(\lambda)$ of its zeros within $(0,\pi)$. Then $N(\lambda) \in \{0,1,2,\ldots\}$, and if $N(\lambda) = i$ then $\lambda_i < \lambda \le \lambda_{i+1}$ holds. If additionally $N(\mu) = i+1$ holds for some $\mu \in \mathbb{R}$ then $\lambda \le \lambda_{i+1} < \mu$. Using bisection, the bounds λ and μ for the i-th eigenvalue of $p(x)$ can be made arbitrarily sharp (see [20, 21] for numerical examples in the case of the potential problem).

If λ_i was known, the i-th eigenfunction $u_i(x)$ of $p(x)$, normalized so that $u_i'(0) = 1$, could be computed by solving the initial value problem (7), with the exact eigenvalue λ_i inserted for λ. In practice, an approximate eigenfunction is computed when an approximate eigenvalue $\tilde{\lambda}_i$ is used in (7).

To normalize the eigenfunctions, the integrals $\int_0^\pi p(x)u_i^2(x)\,dx$ must be evaluated. The elements of the Jacobian are obtained by also evaluating the integrals $\int_0^\pi p_j(x)u_i^2(x)\,dx$ and $\int_0^\pi p_j(x)u_i'^2(x)\,dx$.

4 Inclusion of a solution

If we are interested in guaranteed bounds for the solution of the inverse impedance problem, an infinite iteration of approximate solutions will not do. Therefore, we use interval Newton's method applied to $f(a) = 0$ (where f is defined by (6)) to compute enclosures of a solution of the inverse impedance 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 $[a] = [\underline{a}, \overline{a}]$, $[b] = [\underline{b}, \overline{b}]$, etc. The same notation is used for interval vectors, e.g. $[a] = ([a_j])$. The space of m-dimensional interval vectors is denoted by $I\!R^m$. Real (m, m)-matrices are denoted by $A = (a_{ij})$, the corresponding interval matrices by $[A] = ([a_{ij}])$.

An equation of the form

$$[A][x] \;=\; [b]$$

where $[A]$ is an interval matrix and $[x]$ and $[b]$ are interval vectors is used as a short notation for the set of all linear equations

$$\{\, Ax = b \mid A \in [A],\, b \in [b] \,\}.$$

Following [23], by $[A]^H[b]$ we denote the interval hull of the solution set

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

provided that all $A \in [A]$ are nonsingular. Under certain conditions on $[A]$ and $[b]$, an enclosure of $[A]^H[b]$ can be computed by interval Gaussian elimination ([1, Chap. 15]) or by Krawczyk iteration ([23, Chap. 4.2]). For the sake of simplicity, we denote such an enclosure by LSS($[A]$, $[b]$) (where LSS stands for Linear system Solution Superset), independent of the method that was used to compute it. The choice of the method does not affect the convergence theorem presented below, but it may well affect the speed of convergence in numerical examples.

An *interval function* $[w](x)$ is defined by a pair of continuous functions $\underline{w}$, $\overline{w}$, satisfying $\underline{w}(x) \le \overline{w}(x)$ in $D \subseteq I\!R$:

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

In the following, $p(x; [a])$ stands for a set of linear combinations of the basis functions in the reconstruction procedure, namely

$$\begin{aligned}p(x; [a]) &:= \widehat{p}(x) + \sum_{j=1}^{n} [a_j]\, p_j(x) \\ &:= \{\, \widehat{p}(x) + \sum_{j=1}^{n} a_j\, p_j(x) \mid a_j \in [a_j] \,\}.\end{aligned} \tag{8}$$

It is most important for the implementation of the inclusion procedure that the function set $p(x;[a])$ 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 (8) is possible and yields enclosures of the derivatives of all $p(x) \in p(x;[a])$:

$$\{\, p'(x) \mid p(x) \in p(x;[a]) \,\} \;=\; \widehat{p}'(x) + \sum_{j=1}^{n} [a_j]\, p_j'(x).$$

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 $\dfrac{\partial f_i}{\partial a_j}([a])$, where

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

The interval Newton operator is defined by

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

where $m : I\!R^n \to R^n$, $m([a]) \in [a]$ 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 that if

$$IN([a]) \subseteq [a], \tag{9}$$

then $IN([a])$ encloses a unique zero of f ([23, Chap. 5.2]).

With the above definitions, all computations in Algorithm 1 can be replaced by interval computations. The resulting interval version of our reconstruction procedure is given by Algorithm 2 on the next page.

From the inclusion property (9) of the interval Newton operator, the following theorem is deduced:

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

$$IN([a]^{(k)}) \;\subseteq\; [a]^{(k)}, \tag{10}$$

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

$$p(x;[a]^{(k+1)}) \;=\; \widehat{p}(x) + \sum_{j=1}^{n} [a_j]^{(k+1)} p_j(x)$$

contains exactly one impedance of the form (4), namely

$$p^*(x) \;:=\; p(x;a^*) \;=\; \widehat{p}(x) + \sum_{j=1}^{n} a_j^*\, p_j(x),$$

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

Algorithm 2: Interval Newton's method

1. Choose $[a]^{(0)} \in I\mathbb{R}^n$.
2. For $k = 0, 1, \ldots$:
   (i) For $i = 1, 2, \ldots, n$:
      (a) Compute $f_i(m^{(k)}) = \lambda_i(p_m^{(k)}) - \nu_i$,
      (b) Compute $g_i(x; [a]^{(k)})$,
      where

$$m^{(k)} := m([a]^{(k)}),$$
$$p_m^{(k)}(x) := p(x; m^{(k)}) = \widehat{p}(x) + \sum_{j=1}^{n} m_j^{(k)} p_j(x).$$

   (ii) Compute the Jacobian

$$\left(\frac{\partial f_i}{\partial a_j}([a]^{(k)})\right) = \left(\int_0^\pi \left(g_i'^2(x;[a]) - \lambda_i g_i^2(x;[a])\right) p_j(x)\, dx, \right)_{i,j=1,2,\ldots,n}$$

   (iii) Perform the interval Newton step

$$IN([a]^{(k)}) := m^{(k)} - LSS\left(\left(\frac{\partial f_i}{\partial a_j}([a]^{(k)})\right), f(m^{(k)})\right),$$
$$[a]^{(k+1)} := IN([a]^{(k)}) \cap [a]^{(k)}.$$

When carrying out Algorithm 2 practically, the discretization errors of the numerical integration and the errors due to the stopping of infinite iterations must be included in intervals that enclose eigenvalues, eigenfunctions and the elements of the Jacobian, respectively. This will be discussed in the next two sections.

If the calculations are carried out on a computer, besides discretization errors also roundoff errors must be considered. The latter can be easily handled if there is a reliable computer arithmetic, as it was defined by Kulisch and Miranker in [14], and if programming languages like PASCAL–XSC, C–XSC, or FORTRAN–XSC (cf. [11, 12, 28]) are used. These languages supply a machine interval arithmetic with which the roundoff errors of all arithmetic operations are automatically enclosed in the result. In the following, we assume that this is done in all computations, when executed on a computer.

5 Eigenvalue enclosures

In Section 3, we showed how eigenvalue *approximations* are determined by the shooting method. Similarly, guaranteed eigenvalue *enclosures* can be computed by a modification of the shooting method. It depends on Lohner's enclosure method for the solution of ordinary initial value problems, which Lohner implemented in a PASCAL-XSC program called AWA ([15, 16]). With a modified version of this program, we compute an interval function $[u](x)$ that contains the true solution $u(x)$ of (7).

The computation of eigenvalue bounds is again based on the counting of zeros. In order to count the correct number of zeros, we have to guarantee that whenever the interval function $[u](x)$ crosses the x-axis, $u(x)$ has *exactly one* zero there. To ensure 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 zeros of $u(x)$ are simple, the correct number of zeros can be computed if the function enclosures of the solutions of (7) are sharp enough.

Replacing $p(x; a)$ in (7) by $[p](x) := p(x; [a])$ and applying AWA to the resulting initial value problem, we get simultaneous enclosures of the eigenvalues of all impedances $p(x; a) \in [p](x)$, due to the inclusion monotonicity of the interval operations. To make AWA applicable, $[p](x)$ must be interpreted as a function set in the sense of (8).

6 Eigenfunction enclosures

If an interval $[\lambda]$ is inserted instead of the real parameter λ in the application of AWA to (7), then an interval function $u(x, [\lambda])$ satisfying

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

is computed. This enclosure property is used to procure eigenfunction enclosures for $p(x)$ in two steps:

First, we compute an enclosure $[\lambda_i]$ of the i-th eigenvalue λ_i of $p(x)$. Then we apply AWA to (7) 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 $p(x)$.

Finally, inserting interval data for both $p(x)$ and λ in (7) and applying AWA to the resulting interval initial value problem, we compute an interval function $[u](x) := u(x; [p], [\lambda])$ which satisfies

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

To obtain simultaneous enclosures of the normalized eigenfunctions of all $p(x) \in [p](x)$, we compute an interval $[\lambda_i] \supseteq \{\lambda_i(p) \mid p(x) \in [p](x)\}$ by the method described in the previous section. After that, we apply AWA to (7) to compute the interval function $u(x; [p], [\lambda_i])$ containing the i-th eigenfunctions $u_i(x)$ of all $p(x) \in [p](x)$.

To show how the elements of the Jacobian can be enclosed, we have to give a precise description of the structure of $u(x; [p], [\lambda_i])$. With AWA, the interval $[0, \pi]$ is divided into subintervals $[x_l, x_{l+1}]$, $l = 0, 1, \ldots, l_{max} - 1$. In each subinterval $[x_l, x_{l+1}]$, AWA supplies intervals $[c_k]$, $k = 0, 1, \ldots, r$, that simultaneously enclose the Taylor coefficients up to order $r - 1$ and the corresponding remainder term of $u_i(x) = u(x; p, \lambda_i(p))$ for all $p(x) \in [p](x)$:

$$u_i(x) \ \in \ u(x; [p], [\lambda_i]) \ := \sum_{k=0}^{r} [c_k] \cdot (x - x_l)^k, \quad x \in [x_l, x_{l+1}]. \tag{11}$$

This representation allows us to compute enclosures of squares of eigenfunctions by squaring $u(x;[p],[\lambda_i])$ in each subinterval $[x_l, x_{l+1}] \subset [0,\pi]$ in the form

$$u_i^2(x) \ \in \ \sum_{k=0}^{2r} [d_k] \cdot (x - x_l)^k, \quad x \in [x_l, x_{l+1}]. \tag{12}$$

Similarly, if there is an enclosure of $p(x)$ in the form

$$p(x) \in \sum_{k=0}^{r} [e_k] \cdot (x - x_l)^k, \quad x \in [x_l, x_{l+1}], \tag{13}$$

then by multiplying (12) and (13) we can compute intervals $[f_k]$ so that

$$p(x)u_i^2(x) \ \in \ \sum_{k=0}^{3r} [f_k] \cdot (x - x_l)^k, \quad x \in [x_l, x_{l+1}]. \tag{14}$$

The integral of an interval function $[w](x) = [\underline{w}(x), \overline{w}(x)]$ is defined by

$$\int_a^b [w](x)\, dx := [\int_a^b \underline{w}(x) dx, \int_a^b \overline{w}(x) dx].$$

Since $(x - x_l)^k$ is nonnegative in $[x_l, x_{l+1}]$,

$$[f_k] \cdot (x - x_l) = [\underline{f_k} \cdot (x - x_l), \overline{f_k} \cdot (x - x_l)].$$

Therefore, when integrating (14) we may write the interval coefficients $[f_k]$ before the integral to obtain

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

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

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

yields an enclosure of the normalized eigenfunctions $g_i(x)$ of all $p(x) \in [p](x)$ of the form (11).

Similar enclosures can be obtained for $g_i^2 p_j$ and $g_i'^2 p_j$, if enclosures of the form (11) for all basis functions $p_j(x)$ with the same breakpoints as for the $[g_i](x)$ are provided. In our numerical examples, we used interval functions of this kind to enclose the Jacobian in Algorithm 2 in an interval matrix.

7 Numerical results

Numerically, the reconstruction procedure in this paper appears to be more expensive than the algorithms for approximate solutions given by Knobel and Lowe [13] or Rundell and Sacks [26]. To compute an enclosure of the function value of f and of the Jacobian in Algorithm 2, $2n$ eigenvalue problems have to be solved. The computation of 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.

However, we feel that the effort is justified by the possibility to validate the existence of a solution numerically on the computer. Moreover, 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 approximate real eigenvalues, without modifying a single line of the computer code. With intervals, distinct inverse problems can be solved at the same time, and a sensitivity analysis of the inverse problem is also accomplished.

On the other hand, the standard Rayleigh–Ritz method can be used in a numerically cheap approximate version of our reconstruction procedure. With the approximate eigenvalues and eigenfunctions from the Rayleigh–Ritz method, an approximation of the Jacobian in Algorithm 1 is readily acquired. The complete Algorithm 1 can be performed approximately and the determination of the impedance is essentially reduced to the solution of matrix eigenvalue problems.

In our numerical examples, we used the Rayleigh–Ritz method (with trial functions $\sin(jx)$) to perform the Newton iteration of the reconstruction procedure approximately, until numerical convergence was observed. The resulting approximate solution was then further improved by two or three more steps of Algorithm 1, performed with approximate solution of initial value problems in real machine arithmetic.

An assumed enclosure $[a]^{(0)}$ of a solution of (5), that was used as a starting interval in the interval Newton iteration, was determined from the iterates of the real Newton iteration, using criteria from [2]. With the implementation of Algorithm 2 on a computer, enclosing all roundoff errors in the computation, 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.

In the first approximate iteration steps, however, sometimes the iterated impedance functions became negative, and consequently, the iteration broke down. If this happened, then we damped the particular Newton step by a proper power of $\frac{1}{2}$ to ensure positiveness of the iterates. This worked very well in practice.

As has been pointed out before, the reconstruction of impedance functions with a finite trigonometric series expansion, namely

$$p(x) = \alpha_0 + \sum_{j=1}^{n} \alpha_j \cos(2jx), \quad p(0) = 1, \tag{15}$$

is well defined in a neighborhood of the constant impedance $p(x) = 1$. Instead

of (15) we used the equivalent representation

$$p(x) = 1 + \sum_{j=1}^{n} a_j \sin^2(jx)$$

which has the advantage of fulfilling $p(0) = 1$ automatically. With $p_j(x) = \sin^2(jx)$ and f from (6), at $a^{(0)} = 0$ the Jacobian of f is the nonsingular diagonal matrix with diagonal elements $\dfrac{\partial f_i}{\partial a_i} = -\dfrac{i^2}{2}$.

The reconstruction becomes more and more difficult when the impedance oscillates more rapidly, or when either the infinity norm of the impedance grows larger or the smallest function value tends to zero. In both cases, the eigenvalues behave more and more irregular compared to those of $p = 1$, and therefore $p = 1$ becomes a less and less suitable starting value for Newton iteration. Since the eigenvalues do not change when the impedance is multiplied with a real constant, the condition of the inverse problem can be measured by

$$c(p) := \frac{\max_{[0,\pi]} p(x)}{\min_{[0,\pi]} p(x)}.$$

In the examples presented below, $c(p)$ is always larger than in the examples that were given in [13] and [26].

Our examples were computed using the 16 decimal digit real and interval arithmetic of PASCAL-XSC. Most of the computation time was consumed by the enclosure step. The solutions of the initial value problems (7) were enclosed with a modified version of Lohner's program AWA, adapted to the rather simple structure of the differential equation. The solutions of the linear systems in the interval Newton step where enclosed with the Krawczyk–based PASCAL-XSC problem solving routine LSS [17, Chap. 2.1.5], which is mainly an implementation of the algorithms presented in [25].

Example 1: Verified reconstruction of $p(x) = 1 + 10\sin^2 x$ from 5 eigenvalues

Prescribed eigenvalues: $\nu_1 = 0.277416\ldots$, $\nu_2 = 3.654004\ldots$, $\nu_3 = 9.002180\ldots$, $\nu_4 = 16.27793\ldots$, $\nu_5 = 25.47677\ldots$.

Initial guess: $p^{(0)}(x) = 1$.

Enclosure:

$$\begin{aligned} p(x) \in 1 &+ [\ \ 9.999999999999047\text{E+}000\ ,\ 1.000000000000094\text{E+}001\ ]\ \sin^2 x \\ &+ [\ -2.503\text{E}-013\ ,\ 2.541\text{E}-013\ ]\ \sin^2(2x) \\ &+ [\ -2.016\text{E}-013\ ,\ 2.043\text{E}-013\ ]\ \sin^2(3x) \\ &+ [\ -1.759\text{E}-013\ ,\ 1.692\text{E}-013\ ]\ \sin^2(4x) \\ &+ [\ -1.058\text{E}-013\ ,\ 1.057\text{E}-013\ ]\ \sin^2(5x) \end{aligned}$$

Even though the infinity norm of $p(x)$ is rather large, the reconstruction with Newton's method with starting impedance $p = 1$ is successful, and the bounds from the enclosure step are very tight.

Example 2: Verified reconstruction of $p(x) = 1 + 10\sin^2(5x)$ from 5 eigenvalues

Prescribed eigenvalues: $\nu_1 = 0.543682\ldots$, $\nu_2 = 2.059865\ldots$, $\nu_3 = 4.162909\ldots$, $\nu_4 = 6.113185\ldots$, $\nu_5 = 6.935422\ldots$.

Initial guess: $p^{(0)}(x) = 1 + 9.9\sin^2(5x)$.

Enclosure:

$$\begin{aligned} p(x) \in\ & 1 + [\ -2.238\text{E}{-}012\ ,\ 2.256\text{E}{-}012\ ]\ \sin^2(1x) \\ & + [\ -1.440\text{E}{-}012\ ,\ 1.436\text{E}{-}012\ ]\ \sin^2(2x) \\ & + [\ -1.419\text{E}{-}012\ ,\ 1.423\text{E}{-}012\ ]\ \sin^2(3x) \\ & + [\ -2.153\text{E}{-}012\ ,\ 2.140\text{E}{-}012\ ]\ \sin^2(4x) \\ & + [\ \ 9.999999999992263\text{E}{+}000\ ,\ 1.000000000000777\text{E}{+}001\ ]\ \sin^2(5x) \end{aligned}$$

Again the infinity norm of $p(x)$ is rather large. In this example, $p(x)$ also oscillates rapidly. The eigenvalues have moved towards 0, ν_5 is smaller than even the third eigenvalue of $p(x) = 1$. For the Newton iteration with starting guess $p(x) = 1$, no convergence could be observed within the first 20 iterates. However, for a starting impedance nearer to $1 + 10\sin^2(5x)$, Newton iteration did converge and the enclosure step was also feasible.

Example 3: Verified reconstruction of $p(x) = 1 - 0.9\sin^2(2x)$ from 5 eigenvalues

Prescribed eigenvalues: $\nu_1 = 0.514153\ldots$, $\nu_2 = 9.448701\ldots$, $\nu_3 = 11.64751\ldots$, $\nu_4 = 14.69547\ldots$, $\nu_5 = 28.74919\ldots$.

Initial guess: $p^{(0)}(x) = 1$.

Enclosure:

$$\begin{aligned} p(x) \in\ & 1 + [\ -1.893\text{E}{-}013\ ,\ 1.898\text{E}{-}013\ ]\ \sin^2(1x) \\ & + [\ -9.000000000001002\text{E}{-}001\ ,\ -8.999999999998999\text{E}{-}001\ ]\ \sin^2(2x) \\ & + [\ -5.910\text{E}{-}014\ ,\ 5.928\text{E}{-}014\ ]\ \sin^2(3x) \\ & + [\ -1.712\text{E}{-}014\ ,\ 1.694\text{E}{-}014\ ]\ \sin^2(4x) \\ & + [\ -3.922\text{E}{-}014\ ,\ 3.894\text{E}{-}014\ ]\ \sin^2(5x) \end{aligned}$$

Here, the minimum of the impedance is rather small, namely $p(\frac{\pi}{2}) = 0.1$. But even though ν_2 is larger than the third eigenvalue of $p(x) = 1$, the damped Newton iteration with starting impedance $p(x) = 1$ was convergent.

Example 4: Reconstruction of $p(x) = \left(\cosh x - \tanh(\frac{\pi}{2})\sinh x\right)^2$ from 5 eigenvalues

Prescribed eigenvalues: $\nu_i = i^2 + 1$, $i = 1, \ldots, 5$.

Initial guess: $p^{(0)}(x) = 1$.

The minimum function value of $p(x)$ is about 0.16. With only five eigenvalues, a very good approximation of the impedance function is obtained. To illustrate

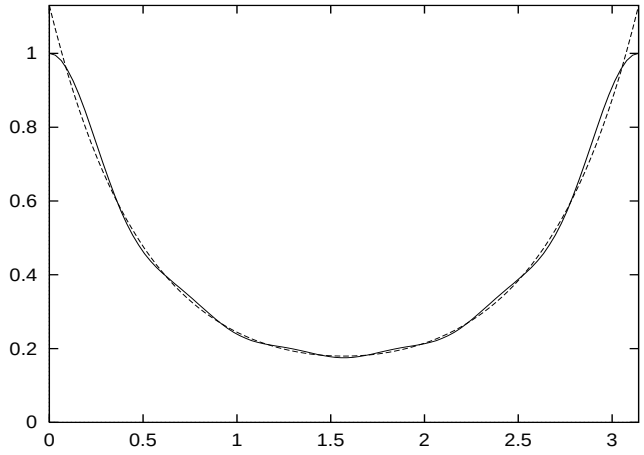

Figure 1: Reconstruction of $p(x) = \left(\cosh x - \tanh(\frac{\pi}{2}) \sinh x\right)^2$

the close resemblance of $p(x)$ and the reconstructed trigonometric approximation, in Figure 1 the latter is plotted against the function $1.13 \cdot p(x)$, which has the same eigenvalues as $p(x)$.

The solution of the inverse impedance problem is not unique, when only finitely many eigenvalues are given. In this example, the enclosure step was feasible and yielded an interval function $[p](x) = [\underline{p}(x), \overline{p}(x)]$ that contains a trigonometric function that has the same first five eigenvalues as the impedance $p(x) = \left(\cosh x - \tanh(\frac{\pi}{2}) \sinh x\right)^2$. The bounds are again very tight, with a maximal value of $\overline{p}(x) - \underline{p}(x)$ of about 1.6E-14.

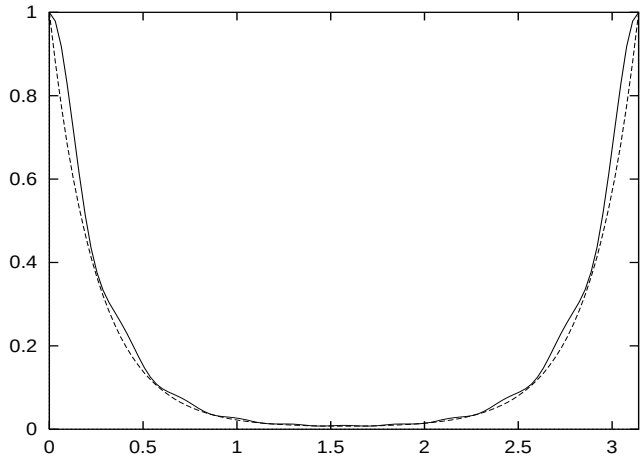

Figure 2: Reconstruction of $p(x) = (\cosh(2x) - \tanh(\pi) \sinh(2x))^2$

Example 5: Reconstruction of $p(x) = (\cosh(2x) - \tanh(\pi)\sinh(2x))^2$ from 10 eigenvalues

Prescribed eigenvalues: $\nu_i = i^2 + 4$, $i = 1, \ldots, 5$.

Initial guess: $p^{(0)}(x) = 1$.

The minimum function value of $p(x)$ is only about 0.0074. But even in this example, an approximation of the impedance was obtained after eight steps of damped Newton iteration. However, the enclosure step was not feasible. With single precision on the computer, the enclosure of the Jacobian was too ill–conditioned.

8 Conclusion

We have presented an enclosure method for the solution of the inverse Sturm–Liouville problem in the impedance case, when finitely many eigenvalues are given for Dirichlet boundary conditions. The method consists of finding a zero of a finite dimensional nonlinear map with Newton's method. In the k-th Newton step, the eigenvalues and eigenfunctions of the iterated impedance function $p^{(k-1)}(x)$ have to be computed.

The approximate version of the reconstruction procedure uses the standard Rayleigh–Ritz method. An approximation of the Jacobian in the Newton iteration is gained from the approximate eigenvalues and eigenfunctions of the Rayleigh–Ritz method, and the determination of the impedance is reduced to the solution of matrix eigenvalue problems.

Applying enclosure principles and interval computations, upper and lower bounds for an impedance that has the given eigenvalues are computed. It is also possible to use eigenvalue intervals instead of real numbers. Thus, distinct inverse problems can be solved simultaneously, and the sensitivity of the inverse problem can also be investigated. With a suitable machine interval arithmetic, the existence of a solution can be validated numerically on the computer.

The practical applicability of the method has been demonstrated with numerical examples. Even for the reconstruction of impedance functions with large infinity norm and rapid oscillations, our method behaves very well.

Acknowledgement: The author would like to thank the anonymous referees for their helpful comments.

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