The Inverse Sturm-Liouville Problem and Finite Differences

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Abstract

In this paper we give a summary of the main results in [Pir92] concerning the inverse Sturm-Liouville problem. We emphasize a convergence result for a Newton method based on finite difference approximation together with a correction technique first introduced by Paine, de Hoog and Anderssen [PdA81].

Keywords: inverse eigenvalue problems, newton method, finite differences

Mathematics Subject Classification: 34B24, 65L12, 65L15, 65L20

1. Introduction. The Sturm-Liouville problem is an eigenvalue problem

$$-y'' + qy = \lambda y, \qquad y, q \in L^2(0,1).$$
 (1)

For simplicity we only consider the boundary value problem with Dirichlet boundary conditions

$$y(0) = y(1) = 0. (2)$$

Thus, the SLP is the problem of finding, given a potential $q \in L^2(0,1)$, a strictly increasing sequence $\underline{\lambda}(q) = (\lambda_1(q), \lambda_2(q), \lambda_3(q), \ldots)$, called the spectrum of q, each value of which satisfies (1) with a corresponding eigenfunction $y \in L^2(0,1)$ satisfying (2).

The inverse Sturm-Liouville problem (ISLP), in which we are particularly interested, can be stated as follows: Given a spectrum $\underline{\lambda}$ of real numbers we want to find a potential q having $\underline{\lambda}$ as its Dirichlet spectrum. Borg, in his fundamental paper [Bor46], was the first to analyse the ISLP. He pointed out that for the case of symmetric potentials, i.e. q(1-x)=q(x), a.e., q is uniquely determined by its spectrum. The question whether the ISLP is well-posed was first partially answered by Hald in [Hal78]. He proved that if two spectra $\underline{\lambda}$ and $\underline{\widetilde{\lambda}}$ are not too far away from the null spectrum $\underline{\lambda}(0)=(k^2\pi^2,k\geq 1)$, i.e. if both numbers $||\underline{\lambda}-\underline{\lambda}(0)||_{l^2}$ and $||\underline{\widetilde{\lambda}}-\underline{\lambda}(0)||_{l^2}$ are sufficiently small, then for the corresponding, uniquely determined, symmetric potentials q and \widetilde{q}

$$||q - \widetilde{q}||_{L^{2}(0,1)} \le S||\underline{\lambda} - \widetilde{\underline{\lambda}}||_{l^{2}} \tag{3}$$

holds for a suitable constant S. An alternative proof for this local well-posedness result with explicit constants is also given in [Pir92, Theorem 4.2.16]. Pöschel and Trubowitz in [PT87] proved well-posedness for the ISLP in the most global context. The spectral data $\underline{\lambda}$ must no longer be near the null spectrum. The remaining conditions are solely $\lambda_1 < \lambda_2 < \cdots$ and

$$\lambda_k = k^2 \pi^2 + s + \alpha_k, \quad s \in \mathbb{R}, \, \underline{\alpha} \in l^2,$$
 (4)

in order that the problem $\underline{\lambda} \to q, q$ symmetric in $L^2(0,1)$, is well-posed. They also gave explicit formulas for the inverse problem. Nonetheless, they did not quantify the Lipschitz constant S of the inverse mapping which makes it difficult to apply their ideas on convergence proofs for numerical

methods, such as finite difference or finite element methods, which also provide faster algorithms for the ISLP.

Numerical methods usually transform the ISLP in a matrix inverse eigenvalue problem. Therefore, many authors worked on properties and algorithms of matrix inverse eigenvalue problems. For a survey of the earlier papers see [Hal72]. A survey of more recent results is given in [BG87]. But many of these discretizations, especially those providing sparse matrices such as finite difference or finite element discretizations, have higher eigenvalues differing significantly from those of the SLP. Consequently, inverse algorithms based on such discretizations either failed completely, when applied on the ISLP, or gave very poor results. In the early Eighties Paine, de Hoog and Anderssen [PdA81] overcame in this context the problem of accurately computing higher SL- eigenvalues by a simple correction technique. They showed, for the case of central difference discretization with an equidistant grid, that even higher SL- eigenvalues can be accurately computed by adding the errors for the null potential – which are explicitly known – to the corresponding eigenvalues of the discretized problem. It turned out that the same correction technique can also be successfully applied to other discretizations, such as Numerov methods [AP85], finite element methods [AP86, Mar90] and multistep methods [VD91].

Based on this correction technique Paine [Pai84] and Marti [Mar90] developed convergent and fast algorithms for the ISLP. But there still was a lack of theory and convergence proofs for such algorithms.

In this paper we want to present a convergence result for an inverse algorithm based on a finite difference discretization with an equidistant grid.

2. Finite Difference Discretization. We discretize the SLP on an equidistant grid $\{x_i : x_i = ih, i = 0, ..., n+1, h=1/(n+1)\}$ and apply central difference discretization on (1), (2). This yields a matrix eigenvalue problem, here called the discrete Sturm-Liouville problem (DSLP),

$$[-A + \operatorname{diag}(q)]\underline{u} = \Lambda \underline{u}, \quad \underline{u} \in \mathbb{R}^n, \tag{5}$$

where $A = h^{-2} \operatorname{tridiag}(1, -2, 1) \in \mathbb{R}^{n \times n}$ and $q_i = q(x_i), i = 1, \dots, n$.

In a first attempt to set up a well-posed discrete inverse eigenvalue problem (DISLP) analogously to the ISLP we may seek, given n real numbers $\Lambda_1 < \Lambda_2 < \cdots < \Lambda_n$, a vector $\underline{q} \in \mathbb{R}^n$ satisfying the symmetry condition $q_i = q_{n+1-i}$, $i = 1, \ldots, n$, (henceforth called a *symmetric* vector) and having $\underline{\Lambda} = (\Lambda_1, \dots, \Lambda_n)^T$ as its DSL- spectrum. A simple comparison of dimensions yields that the DISLP stated as above cannot be well-posed. As a necessary condition for well-posedness of the DISLP the dimensions of the underlying domain and the range of the mapping must be equal.

In fact, the full DSL- spectrum contains, in a sense, too much information (although this seems to be a paradox at the first glance); namely information of both the SL- spectrum of the potential q and of -q, as has been shown in [Pir92, Theorem 2.2.8]:

Proposition 1 For the DSL- eigenvalues of (5) we have

$$\Lambda_k(-\underline{q}) = \frac{4}{h^2} - \Lambda_{n+1-k}(\underline{q}) \quad k = 1, \dots, n.$$

We thus modify our DISLP as follows: Let n=2m be even. Given m=n/2 numbers $\Lambda_1 < \Lambda_2 < \cdots < \Lambda_m$ we seek a symmetric vector $\underline{q} \in \mathbb{R}^n$ (i.e. satisfying the symmetry condition $q_i=q_{n+1-i}, i=1,\ldots,n$) having $\Lambda_1,\ldots,\Lambda_m$ as lowest m values in its DSL- spectrum.

3. Well-posedness for the DISLP. In order to be consistent with (3) we define the discrete L^2 - norm for $q \in \mathbb{R}^n$ by

$$||\underline{q}||_h := \sqrt{h\underline{q}^T\underline{q}}.$$

For the DISLP the l^2 - norm has to be replaced by the 2- norm $\|\cdot\|_{\mathbb{R}^m}$ in \mathbb{R}^m . Having in mind that

$$\Lambda_k(\underline{0}) = \frac{4}{h^2} \sin^2\left(k\pi \frac{h}{2}\right), \quad k = 1, \dots, n,$$

we may state our well-posedness result for the DISLP analogously to (3) and $(4)^{\dagger}$:

Theorem 1 Let n = 2m and the given half spectrum $\Lambda_1 < \Lambda_2 < \cdots < \Lambda_m$ shall satisfy the condition

$$\|\underline{\Lambda} - \underline{\Lambda}(\underline{0})\|_{\mathbb{R}^m} \le \rho, \quad \text{with } \rho = 0.0091,$$
 (6)

[†] For the DISLP we set s, the spectral shift, to zero. The case with arbitrary spectral shift s makes no difficulties and can be treated analogously.

then the DISLP is well-posed.

More precisely, if $\widetilde{\Lambda}_1 < \cdots < \widetilde{\Lambda}_m$ is another half spectrum satisfying (6) then $\underline{\Lambda}$ and $\underline{\widetilde{\Lambda}}$ are the DSL- half spectra of two uniquely determined symmetric vectors $\underline{q}, \underline{\widetilde{q}} \in \mathbb{R}^n$ having discrete L^2 - norms $\leq R = 0.0259$ and satisfying the inequality

$$\|\underline{q} - \underline{\widetilde{q}}\|_h \le 2\sqrt{2}\|\underline{\Lambda} - \underline{\widetilde{\Lambda}}\|_{\mathbb{R}^m}.$$
 (7)

This result is proven in [Pir92, Theorem 4.3.17].

We shall refer to (7) as the stability equation of the DISLP with stability constant $S = 2\sqrt{2}$ and stability thresholds R and $\rho = R/S$. It is a crucial point, in order to prove convergence for algorithms based on the DISLP, that the constants S, R and ρ are independent of the grid size h and that the discrete norms converge, in the limit, to the norms (i.e L^2 - norm and l^2 - norm) considered in the ISLP. For further information on this problem in nonlinear stability see also [Ste73], [Kel75], [LMSS88a], [LMSS88b] or [Pir91].

4. A Newton Method for the DISLP. Given a half spectrum $\underline{\Lambda} \in \mathbb{R}^m$ we want to find symmetric solutions $q \in \mathbb{R}^n$, n = 2m, of the equation

$$F(\underline{q}) = \begin{bmatrix} \Lambda_1(\underline{q}) & - & \Lambda_1 \\ & \vdots & \\ \Lambda_m(q) & - & \Lambda_m \end{bmatrix} = \underline{0}, \tag{8}$$

where $\underline{\Lambda}(\underline{q})$ is the half spectrum of the DSLP (5). The Newton method for the half spectrum was first proposed by Hald [Hal72, p.151]. It yields a sequence of symmetric vectors $q^{(j)} \in \mathbb{R}^n$ satisfying

$$\left[\underline{q}^{(j+1)}\right]_{m} = \left[\underline{q}^{(j)}\right]_{m} - \left[\frac{\partial F(\underline{q}^{(j)})}{\partial [q]_{m}}\right]^{-1} F(\underline{q}^{(j)}), \quad j = 1, 2, \dots$$
(9)

Here $[\cdot]_m : \mathbb{R}^{2m} \to \mathbb{R}^m$ denotes the canonical projection defined by $[\underline{q}]_m := (q_1, \ldots, q_m)^{T\dagger}$. The partial derivatives can be easily computed from the eigenvectors $\underline{u}_{\cdot,k}(\underline{q}) \in \mathbb{R}^n$ of (5): $\partial F_k/\partial \underline{q}_j = 2\underline{u}_{jk}^2(\underline{q}), j, k = 1, \ldots, m$, (see [Hal72,

[†] Clearly, in reverse, every vector $[\underline{q}]_m \in \mathbb{R}^m$ can be extended to a unique symmetric vector $q \in \mathbb{R}^{2m}$.

p.141] or [Pir92, p.9]). However, we still do not know whether the Jacobian $\partial F/\partial \underline{q}$ is always invertible according to a conjecture of Hald [Hal72, p.145]. But now, we know it for small potentials by the stability inequality (7). In addition, we have:

Theorem 2 Let $\underline{\Lambda} \in \mathbb{R}^m$, n = 2m, be a half spectrum satisfying the condition (6) of Theorem 1 with stability threshold $\rho = 0.0091/2$. Then, for every choice of the initial symmetric vector $\underline{q}^{(0)} \in \mathbb{R}^n$ with discrete L^2 -norm $\leq R = 0.0259$, the sequence $\underline{q}^{(j)}$ of (9) is well-defined and converges quadratically, in the discrete L^2 -norm, to a symmetric vector $\underline{q} \in \mathbb{R}^n$. The vector \underline{q} is the unique symmetric solution of (8) with discrete L^2 -norm $\leq R/2$.

The proof is essentially the same as in [Pir92, Theorem 4.3.20].

5. Consistency and Rate of Convergence. Now the question that arises is: Can the Newton method for the DISLP also provide an algorithm for the ISLP? In other words: Can the solutions \underline{q} of (8) converge, in a sense which has to be specified, to a true solution q of the ISLP?

The data of the ISLP are a spectrum $\underline{\lambda}$ satisfying the asymptotic condition (4)[†]. But the data for DISLP, in order to be well–posed, have to satisfy the asymptotic condition (6) of Theorem 1 which reads

$$\Lambda_k \approx \frac{4}{h^2} \sin^2\left(k\pi \frac{h}{2}\right), \quad \text{for } k \text{ large enough.}^{\dagger\dagger}$$
(10)

Since the two asymptotics are not the same the data for the DISLP must be adjusted. And it is exactly the correction technique introduced in [PdA81], performed in reverse, which does this adjustment. Thus, the half spectrum $\underline{\Lambda}$ of F in (8) must be defined as

$$\Lambda_k = \lambda_k - k^2 \pi^2 + \frac{4}{h^2} \sin^2 \left(k \pi \frac{h}{2} \right), \quad k = 1, \dots, m.$$
(11)

Now the data $\underline{\Lambda}$ are consistent with condition (10) and our Newton method may be applied.

[†] Again, for simplicity, we set the spectral shift s = 0.

^{††} For more details on this subject see [Pir92, DSL-Counting-Lemma, Theorem 3.5.1 and Korollar 3.5.7].

Definition 1 A sequence of vectors $\underline{q}^{(m)} \in \mathbb{R}^{2m}$ is said to be convergent to an element $q \in L^2(0,1)$ iff

$$||\underline{q}^{(m)} - (q)_h||_h \to 0, \quad as \quad m \to \infty,$$

where $(q)_h := (q(x_1), q(x_2), \dots, q(x_{2m}))^T$.

Together with this definition, we may now state our main theorem:

Theorem 3 Let the data $\underline{\lambda}$ of the ISLP satisfy the condition $||\underline{\lambda} - \underline{\lambda}(0)||_{l^2} \leq \rho = 0.0091/2$ and belong to a solution $q \in L^2(0,1)$ being twice continuously differentiable. In addition, let the data $\underline{\Lambda}$ for (8) be corrected according to (11). Then the Newton method (9) supplies uniquely determined approximations $\underline{q}^{(m)} \in \mathbb{R}^{2m}$, m sufficiently large, which converge to the solution q with order not smaller than 1/2, i.e.

$$\|\underline{q}^{(m)} - (q)_h\|_h = O(\sqrt{h}).$$

Proof. Let $\underline{\lambda}$ be a SL- spectrum and $\underline{\Lambda}$ be the half spectrum corrected according to (11). For a continuous potential q we introduce the truncation error

$$\tau_{h}(q) := F((\underline{q})_{h}) - \begin{bmatrix} \lambda_{1}(q) - \lambda_{1} \\ \vdots \\ \lambda_{m}(q) - \lambda_{m} \end{bmatrix} = \begin{bmatrix} \Lambda_{1}((q)_{h}) - \lambda_{1}(q) - \Lambda_{1}(\underline{0}) + \lambda_{1}(0) \\ \vdots \\ \Lambda_{m}((q)_{h}) - \lambda_{m}(q) - \Lambda_{m}(\underline{0}) + \lambda_{m}(0) \end{bmatrix}.$$

We may now apply the result of Paine, de Hoog and Anderssen [PdA81] which states that for q twice continuously differentiable

$$\tau_h(q)_k = O(kh^2) \le Mkh^2, \quad k = 1, \dots, m,$$
 (12)

where the constant $M = M(\|q\|_{\infty}, \|q'\|_{\infty}, \|q''\|_{\infty})$ depends on q but not on k or h. It follows immediately that

$$\|\tau_h(q)\|_{\mathbb{R}^m} = \left[\sum_{k=1}^m \tau_h(q)_k^2\right]^{1/2} \le M\sqrt{h}.$$

Now let q be a twice continuously differentiable solution of the ISLP. Our truncation error then reduces to $\tau_h(q) = \underline{\Lambda}((q)_h) - \underline{\Lambda}$. We have

$$\|\underline{\Lambda} - \underline{\Lambda}(\underline{0})\|_{\mathbb{R}^m} \le \|\lambda - \lambda(0)\|_{l^2} \le \rho$$
.

In addition, $\|\underline{\Lambda}((q)_h - \underline{\Lambda})\|_{\mathbb{R}^m} \leq \|\underline{\Lambda} - \underline{\Lambda}(\underline{0})\|_{\mathbb{R}^m} + \|\tau_h(q)\|_{\mathbb{R}^m} \leq \rho + M\sqrt{h}$. Thus, for h sufficiently small, both Theorem 1 and Theorem 2 apply. The stability inequality (7) yields

$$\|\underline{q}^{(m)} - (q)_h\|_h \le 2\sqrt{2}\|F(\underline{q}^{(m)}) - F((\underline{q})_h)\|_{\mathbb{R}^m} = 2\sqrt{2}\|\tau_h(q)\|_{\mathbb{R}^m} = O(\sqrt{h}),$$

since $F(q^{(m)}) = \underline{0}$. This completes our proof.

6. Numerical experiments. Our Newton method has been tested in three qualitatively different examples and with different L^2 - norms R of the solution q of the ISLP (see next three pages[†]). The data $\underline{\lambda}$ of the ISLP have been computed, from the solution q, with a Galerkin method that yields good approximations for the SL- eigenvalues (see [Pir92, Kapitel 5]).

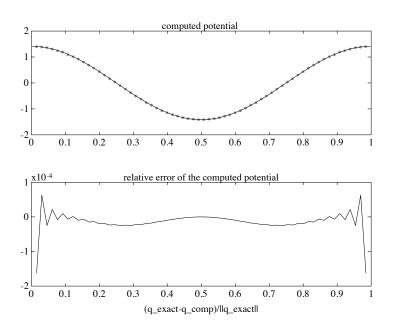
In Example 1 the solution

$$q(x) = R\sqrt{2}\cos 2\pi x \,, \quad 0 \le x \le 1,$$

is the potential of the *Mathieu equation* and is infinitely often differentiable. In *Example 2* the solution q has a discontinuous first derivative and in *Example 3 q* is discontinuous itself. In all three examples the parameter R denotes the L^2 - norm of the solution q. We see that in all three cases the Newton method yields good approximations even if q is large. For *Example 1* and *Example 2* the observed order of convergence is 1.5. This is not too surprising, since one can also observe that in (12) the error term $O(kh^2)$ is not strict. We rather have an $O(h^2)$ error (a observation which is still unproven) which implies this order of convergence.

 $^{^{\}dagger}$ We henceforth omit subscripts for the $\it L^2-$ norm.

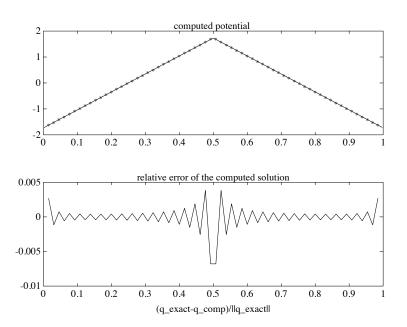
Example 1. Plot for R = 1, m = 32, h = 1/65:



Further results for Example 1:

Further results for Example 1:				
m	Newton steps	$err := q_{\text{comp}} - q_{\text{exact}} _{\mathbf{h}}/R$	$err/h^{1.5}$	
Numerical values for $R = q_{\text{exact}} = 1$:				
2	2	$4.05967 \cdot 10^{-3}$	$4.53877 \cdot 10^{-2}$	
4	3	$9.38247 \cdot 10^{-4}$	$2.53327 \cdot 10^{-2}$	
8	3	$3.00717 \cdot 10^{-4}$	$2.10780 \cdot 10^{-2}$	
16	3	$1.00799 \cdot 10^{-4}$	$1.91086 \cdot 10^{-2}$	
32	3	$3.42074\cdot 10^{-5}$	$1.79263 \cdot 10^{-2}$	
64	3	$1.76485 \cdot 10^{-5}$	$1.72374 \cdot 10^{-2}$	
Numerical values for $R = q_{\text{exact}} = 25$:				
2	5	$4.11258 \cdot 10^{-1}$	$4.59801 \cdot 10^{-0}$	
4	4	$2.75162 \cdot 10^{-2}$	$7.42938 \cdot 10^{-1}$	
8	4	$7.79034 \cdot 10^{-3}$	$5.46047 \cdot 10^{-1}$	
16	4	$2.53686 \cdot 10^{-3}$	$4.80914 \cdot 10^{-1}$	
32	4	$8.54439 \cdot 10^{-4}$	$4.47766 \cdot 10^{-1}$	
64	4	$2.93570 \cdot 10^{-4}$	$4.30126 \cdot 10^{-1}$	

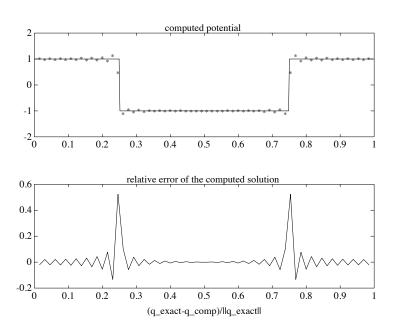
Example 2. Plot for R = 1, m = 32, h = 1/65:



Further results for Example 2:

Further results for Example 2.					
m	Newton steps	$err := q_{\text{comp}} - q_{\text{exact}} _{\mathbf{h}}/R$	$err/h^{1.5}$		
Numerical values for $R = q_{\text{exact}} = 1$:					
2	2	$7.98441 \cdot 10^{-2}$	$8.92684 \cdot 10^{-1}$		
4	3	$3.40742 \cdot 10^{-2}$	$9.20004 \cdot 10^{-1}$		
8	3	$1.29612 \cdot 10^{-2}$	$9.08486 \cdot 10^{-1}$		
16	3	$4.70356 \cdot 10^{-3}$	$8.91656 \cdot 10^{-1}$		
32	3	$1.67895 \cdot 10^{-3}$	$8.79848 \cdot 10^{-1}$		
64	3	$5.95863 \cdot 10^{-4}$	$8.73034 \cdot 10^{-1}$		
Numerical values for $R = q_{\text{exact}} = 25$:					
2	4	$1.27800 \cdot 10^{-1}$	$1.54065 \cdot 10^{-0}$		
4	4	$3.55341 \cdot 10^{-2}$	$9.59420 \cdot 10^{-1}$		
8	5	$1.27161 \cdot 10^{-2}$	$8.91391 \cdot 10^{-1}$		
16	4	$4.63696 \cdot 10^{-3}$	$8.79031 \cdot 10^{-1}$		
32	4	$1.65700 \cdot 10^{-3}$	$8.68343 \cdot 10^{-1}$		
64	4	$5.86915 \cdot 10^{-4}$	$8.59924 \cdot 10^{-1}$		

Example 3. Plot for R = 1, m = 32, h = 1/65:



Further results for Example 3:

Further results for Example 5:				
m	Newton steps	$err := q_{\text{comp}} - q_{\text{exact}} _{\text{h}}/R$	$err/h^{0.5}$	
Numerical values for $R = q_{\text{exact}} = 1$:				
2	2	$3.83697 \cdot 10^{-1}$	$8.57972 \cdot 10^{-1}$	
4	3	$2.82619 \cdot 10^{-1}$	$8.47858 \cdot 10^{-1}$	
8	3	$2.01128 \cdot 10^{-1}$	$8.29273 \cdot 10^{-1}$	
16	3	$1.42035 \cdot 10^{-1}$	$8.15928 \cdot 10^{-1}$	
32	3	$1.00246 \cdot 10^{-1}$	$8.08207 \cdot 10^{-1}$	
64	3	$7.07968 \cdot 10^{-2}$	$8.04097 \cdot 10^{-1}$	
Numerical values for $R = q_{\text{exact}} = 25$:				
2	4	$2.87705 \cdot 10^{-1}$	$6.43328 \cdot 10^{-1}$	
4	4	$2.65356 \cdot 10^{-1}$	$7.96068 \cdot 10^{-1}$	
8	4	$1.90924 \cdot 10^{-1}$	$7.87199 \cdot 10^{-1}$	
16	4	$1.36622 \cdot 10^{-1}$	$7.84833 \cdot 10^{-1}$	
32	4	$9.78500 \cdot 10^{-2}$	$7.88892 \cdot 10^{-1}$	
64	4	$6.98430 \cdot 10^{-2}$	$7.93264 \cdot 10^{-1}$	

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