An inversion algorithm for recovering a coefficient of Sturm-Liouville operator

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Abstract

In this paper, an efficient algorithm for recovering a density of Sturm-Liouville operator from given two spectra is investigated. Based on Lidskii's theorem and Mercer's theorem, we build a sequence of trace formulae which bridge explicitly the density and eigenvalues in terms of nonlinear Fredholm integral equations. Due to intrinsic difficulties on ill-posedness of an inverse spectral problem, a truncated Fourier series regularization method is utilized for reconstructing the unknown density. Moreover, shifted Legendre polynomials are carried to balance the different order of trace formulae. Numerical results are presented to illustrated the effectiveness and stability of the proposed reconstruction algorithm.

AMS(MOS) subject classification: 45C05, 34L16

Keywords. Invesre Sturm-Liouville Problem, Trace formulae, Line search Newton-like Method

1 Introduction

We are concerned with a Sturm-Liouville equation

$$-\frac{d^2u}{dx^2} = \lambda\rho(x)u,\tag{1.1}$$

with two separated boundary conditions (BCs)

$$\sin(a)u(0) + \cos(a)u'(0) = 0, \tag{1.2}$$

$$\sin(b)u(1) + \cos(b)u'(1) = 0, \tag{1.3}$$

where the density $\rho(x)$ is a positive and unknown function defined in the interval [0, 1] and the coefficients $a, b \in [0, \pi)$.

Our interest in this paper lies in computing the density function ρ everywhere on the interval [0, 1] from two spectra. Let

$$\{\lambda_{1,k}(\rho, a, b)\}_{k=1,2,\dots}$$
(1.4)

be a first spectrum of the equation (1.1) with Dirichlet-Dirichlet boundary conditions (DDBCs), i.e., $a = b = \pi/2$, and

$$\{\lambda_{2,k}(\rho, a, \hat{b})\}_{k=1,2,\dots}, \quad \hat{b} \neq b$$
(1.5)

a second spectrum corresponding to Dirichlet-Neumann boundary conditions (DNBCs), i.e., $a = \pi/2$, $\hat{b} = 0$. Besides, these two spectra (1.4) and (1.5) are assumed to be arranged from small to large according to

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their values. In 1946, Borg [6] proved that two spectrum can uniquely determine the density of a string equation. Actually, if $\rho \in C^2([0, 1])$, then with the following Liouville transformation [19, 20]

$$\begin{cases} c = \int_0^1 \sqrt{\rho(t)} dt, \\ \xi = \int_0^x \sqrt{\rho(t)} dt, \\ y(\xi) = \rho^{1/4}(x)u(x), \\ q(\xi) = \rho^{-1/4}(x) \frac{d^2}{dx^2} \rho^{1/4}(x) \end{cases}$$

the equation (1.1) reduces to a second-order Sturm-Liouville equation with potential function q over [0, c] of the form

$$-y''(\xi) + q(\xi)y(\xi) = \lambda y(\xi).$$
(1.6)

Together with some boundary conditions, the numerical method of inverse Sturm-Liouville problem (SLP) for recovering the potential function q in (1.6) had been studied intensively in past two decades. Theoretically, Sini [21] reviewed four popular methods, i.e., the asymptotic expansion technique, the integral equation technique, the C-priperty and the boundary control method, for proving the uniqueness results of inverse SLP. Numerically, Sacks [18] described several computational methods, i.e., the integral equation method, optimization method and matrix method, to recover q from spectral data. In terms of a single given spectrum, a potential q which is even with respect to x = c/2 [2, 7, 9, 13] or is given over the interval [c/2, c] [1, 3, 14] can be reconstructed. For the case of providing two-spectrum, the main methods of recovering general potentials are iteration approaches [4, 5, 8, 16, 17]. The primary differences are in the way of determining eigenvalues on direct problem or optimization methods on inverse problem. Rundell and Sacks [17] proposed a transformation method using a reference potential which results in solving a hyperbolic partial differential equation in each iteration step. Andrew [4] applied Numerov's method to approximate the eigenvalues in each modified Newton's iteration for recovering a non-symmetric potential. Gao et al. [8] using a boundary value method (BVM) [10] as the main tool for estimating the eigenvalues in each Newton iteration step. Böckmann and Kammanee [5] proposed a derivative-free method for recovering symmetric and non-symmetric potential functions in each Broyden iteration step. The methods mentioned above all rely heavily on the accuracy and the computing speed of direct problem.

Current work is a direct extension of Xu and Zhai [22], where an explicit relationship between the trace operator and given eigenvalues $\{\lambda_k\}_{k=1}^{\infty}$ was derived through the Lidskii's theorem, i.e.,

$$\operatorname{trace}(K) = \sum_{k=1}^{\infty} \lambda_k^{-1}.$$
(1.7)

For the sake of keeping inverse on of the above trace formula (1.7) being stable, we choose different orthogonal polynomials from [22], i.e., shifted Legendre polynomials to convert the relationship (1.7) into

$$\operatorname{trace}(\tilde{L}_n(K)) = \sum_{k=1}^{\infty} \tilde{L}_n(\lambda_k^{-1}).$$
(1.8)

With the truncated Fourier series regularization method and the function of scaling factors, we finally obtain a system of trace formulae which could be solved by line search Newton-like method [12, 23]. A line-search method may not be able to achieve sufficient decrease, whereas the step length that satisfies the Wolfe conditions [11] is designed to guarantee a reasonable convergence property.

This paper is organized as follows. A brief introduction about Numerov's method to solve the forward problem is given in Section 2. Subsequently, Sections 3 deals with the inverse problem by using the trace formulae. Afterwards, we discuss the inversion algorithm for recovering the density in Section 4. Finally, in Section 5, numerical examples with non-symmetric density functions demonstrate effectiveness of the proposed reconstruction method.

2 Numerov's method for the direct problem

In this section, for completeness, we briefly recall the Numerov's method introduced in [2, 15] for approximations of eigenvalues of the SLP (1.1)-(1.3). This method is based on the application of finite difference methods for the solution of ODEs over an assigned partition of [0, 1] frequently composed by

$$x_i = ih, \ i = 0, 1, \dots, N+1, \ h = \frac{1}{N+1}.$$

Denote $u(x_i)$ by u_i and $\rho(x_i)$ by ρ_i . Recall Taylor's expansion of the following functions

$$u_{i+1} = u(x_i + h) = u_i + hu'_i + \frac{h^2}{2!}u''_i + \frac{h^3}{3!}u'''_i + \frac{h^4}{4!}u_i^{(4)} + \cdots$$
(2.1)

$$u_{i-1} = u(x_i - h) = u_i - hu'_i + \frac{h^2}{2!}u''_i - \frac{h^3}{3!}u''_i + \frac{h^4}{4!}u_i^{(4)} + \cdots$$
(2.2)

From Eqs (2.1) and (2.2), it follows that

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = u_i'' + \frac{h^2}{12}u_i^{(4)} + O(h^4).$$
(2.3)

As $u^{(4)} = (-\lambda \rho u)''$, substituting u'' and $u^{(4)}$ into (2.3) and applying difference approximation yield

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} = -\frac{1}{12}\lambda(\rho_{i+1}u_{i+1} + 10\rho_iu_i + \rho_{i-1}u_{i-1})$$
(2.4)

with local truncation error $O(h^2)$. Now using the same idea as in finite difference method, it gives

$$A\boldsymbol{u} = -\lambda B\boldsymbol{u},\tag{2.5}$$

where $A = (1/h^2)T$, $B = (I + \frac{1}{12}T)Q$. In addition, $Q = diag(\rho_1, \rho_2, ..., \rho_N)$, and

$$T = \begin{pmatrix} T_{11} & 1 & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & T_{NN} \end{pmatrix}_{N \times N}$$

with $T_{11} = -2 + \frac{1}{1 - \frac{\sin(a)}{\cos(a)}h}$, $T_{NN} = -2 + \frac{1}{1 + \frac{\sin(b)}{\cos(b)}h}$ for the boundary conditions (1.2) and (1.3).

3 Trace formulae for the inverse problem

In this section, we will determin the density $\rho(x)$ in (1.1) from two spectra (1.4) and (1.5), which are corresponding to the SLP with DDBCs and DNBCs respectively. Note that $\rho(x)$ in (1.1) is uniquely determined from two spectra (1.4) and (1.5). As a result, we refer to this problem as the DD-DN inverse problem.

The solution of problem (1.1)-(1.3) can be expressed in the form of

$$u(x) = \lambda \int_0^1 \rho(y)g(x,y)u(y)dy, \qquad (3.1)$$

where

$$g(x,y) = g_1(x,y) = \begin{cases} x(1-y), & 0 \le x \le y \le 1, \\ y(1-x), & 0 \le y \le x \le 1 \end{cases}$$

for Dirichlet-Dirichlet BCs and

$$g(x,y) = g_2(x,y) = \begin{cases} x, & 0 \le x \le y \le 1, \\ y, & 0 \le y \le x \le 1 \end{cases}$$

for Dirichlet-Neumann BCs.

Denoting the operator K as $Ku = \int_0^1 \rho(y)g(x,y)u(y)dy$, we have

$$Ku = \lambda^{-1}u. \tag{3.2}$$

As K is a bounded linear operator over a separable Hilbert space, from the Lidskii's theorem, we have

$$\operatorname{trace}(K) = \sum_{k} \Lambda_k(K), \qquad (3.3)$$

where $\{\Lambda_k(K)\}\$ are the eigenvalues of K. Clearly,

$$\sum_{k} \Lambda_k(K) = \sum_{k=1}^{\infty} \lambda_k^{-1}, \qquad (3.4)$$

which provides, with the proposition 2 introduced in [22], the representation of trace(K),

$$\operatorname{trace}(K) = \int_0^1 \rho(x)g(x,x)dx. \tag{3.5}$$

Define the trace of K^s , $s \in \mathbb{Z}^+$ as

$$\tau_s(\rho) = \operatorname{trace}(K^s). \tag{3.6}$$

obviously $\tau_s(\rho) = \sum_{k=1}^{\infty} \lambda_k^{-s}$. By proposition 1 and proposition 2 presented in [22], we have

$$\tau_s(\rho) = \int_0^1 \cdots \int_0^1 \rho(x_1) g(x_1, x_2) \cdots \rho(x_s) g(x_s, x_1) dx_1 \cdots dx_s.$$
(3.7)

Consequently, we build a relationship between the function ρ and the given data λ . Especially, we have the following two trace formulae

$$\sum_{k=1}^{\infty} \lambda_{1,k}^{-s_1} = \int_0^1 \cdots \int_0^1 \rho(x_1) g_1(x_1, x_2) \cdots \rho(x_{s_1}) g_1(x_{s_1}, x_1) dx_1 \cdots dx_{s_1}, \ s_1 \in \mathbb{Z}^+$$
(3.8)

for Dirichlet-Dirichlet BCs and

$$\sum_{k=1}^{\infty} \lambda_{2,k}^{-s_2} = \int_0^1 \cdots \int_0^1 \rho(x_1) g_2(x_1, x_2) \cdots \rho(x_{s_2}) g_2(x_{s_2}, x_1) dx_1 \cdots dx_{s_2}, \ s_2 \in \mathbb{Z}^+$$
(3.9)

for Dirichlet-Neumann BCs.

4 Inversion algorithm

The following theorem will be utilized to design a inversion algorithm later.

Theorem 4.1 (Mercer's theorem) Assume an operator K is positive definite, and its associated kernel K(x, y) is a real-valued symmetric, continuous function of x and y. Then K can be expanded in a uniformly convergent series

$$K(x,y) = \sum_{n=1}^{\infty} \nu_n \varphi_n(x) \varphi_n(y),$$

where ν_n and φ_n are the eigenvalues and normalized eigenfunctions of K.

Assume $\{\mu_n, \phi_n(x)\}_{n=1}^{\infty}$ are the eigenvalues and normalized eigenfunctions of $-\Delta$, where

$$-\Delta\phi_n = -\phi_n'' = \mu_n\phi_n.$$

Applying Mercer's theorem to $(-\Delta)^{-1}$ whose kernel is g(x, y), we have

$$g(x,y) = \sum_{n=1}^{\infty} \mu_n^{-1} \phi_n(x) \phi_n(y).$$
(4.1)

Substituting (4.1) into (3.7), it's easy to see that

$$\tau_s(\rho) = \sum_{n_1,\cdots,n_s} \frac{1}{\mu_{n_1}\cdots\mu_{n_s}} \left(\int_0^1 \phi_{n_1}(x)\phi_{n_2}(x)\rho(x)dx \right) \times \cdots \times \left(\int_0^1 \phi_{n_s}(x)\phi_{n_1}(x)\rho(x)dx \right).$$

Denote $\mathbf{M}(\rho)$ to be an infinite-dimensional matrix where the element of the *i*th line and *j*th column

$$\mathbf{M}_{ij}(\rho) = \frac{1}{\sqrt{\mu_i \mu_j}} \int_0^1 \phi_i(x) \phi_j(x) dx.$$
(4.2)

Then we have

$$\sum_{k=1}^{\infty} \lambda_k^{-s} = \tau_s(\rho) = \operatorname{trace}(\mathbf{M}^s(\rho)).$$
(4.3)

4.1 Trigonometric polynomial

It's natural to approximate the density function ρ by the following basis functions

$$\psi_{2m-1}(x) = \cos(2(m-1)\pi x), \ \psi_{2m}(x) = \sin(2m\pi x) \ m = 1, 2, \dots, M.$$

The corresponding best approximation, in L^2 -norm, of the density, given by

$$\rho(x) = \sum_{m=1}^{2M} a_m \psi_m(x), \ a_m(x) = \frac{\int_0^1 \rho(x) \psi_m(x) dx}{\int_0^1 \psi_m^2(x) dx}$$
(4.4)

is the truncated Fourier series of the periodic extension of ρ with period 1. However, that if ρ is sufficiently regular, the error with respect to such best approximation decreases as $O(M^{-1/2})[1]$. It is prefered to consider the space with basis functions given by

$$\psi_m(x) = \cos((m-1)\pi x), \ m = 1, 2, \dots, 2M.$$
 (4.5)

And denote $\mathbf{a} = \{a_1, a_2, \cdots, a_{2M}\}$. We use $\tau_s(\mathbf{a}), \mathbf{M}(\mathbf{a})$ in place of $\tau_s(\rho), \mathbf{M}(\rho)$. Then

$$\mathbf{M}_{ij}(\mathbf{a}) = \sum_{m=1}^{2M} a_m \mathbf{M}_{ij}(\mathbf{e}_m), \tag{4.6}$$

where $\mathbf{M}_{ij}(\mathbf{e}_m) = \frac{1}{\sqrt{\mu_i \mu_j}} \int_0^1 \phi_i(x) \phi_j(x) \psi_m(x) dx$, and $\mathbf{e}_m = \{a_1 = 0, \cdots, a_{m-1} = 0, a_m = 1, a_{m+1} = 0, \cdots, a_{2M} = 0\}$.

For the case of Dirichlet-Dirichlet BCs, the eigenvalues $\mu_n = n^2 \pi^2$ and the eigenfunctions $\psi_n(x) = \sqrt{2} \sin n\pi x$. Therefore,

$$\begin{split} \mathbf{M}_{ij}(\mathbf{e}_m) &= \mathbf{M}_{ij}^{(1)}(\mathbf{e}_m) &= \frac{2}{\pi^2 i j} \int_0^1 \sin i \pi x \sin j \pi x \cos(m-1) \pi x dx \\ &= \begin{cases} -\frac{1}{2\pi^2 i j}, & i+j+m-1=0, \\ -\frac{1}{2\pi^2 i j}, & i+j-m+1=0, \\ \frac{1}{2\pi^2 i j}, & i-j+m-1=0, \ m \neq 1, \\ \frac{1}{2\pi^2 i j}, & i-j-m+1=0, \ m \neq 1, \\ \frac{\pi^2 i j}{\pi^2 i j}, & i=j, \ m=1, \\ 0, & \text{otherwise.} \end{cases} \end{split}$$

Similarly, for the case of Dirichlet-Neumann BCs, the eigenvalues $\mu_n = \left(\frac{2n-1}{2}\pi\right)^2$, the eigenfunctions $\psi_n(x) = \sqrt{2} \sin \frac{2n-1}{2}\pi x$, and

$$\begin{split} \mathbf{M}_{ij}(\mathbf{e}_m) &= \mathbf{M}_{ij}^{(2)}(\mathbf{e}_m) &= \frac{8}{\pi^2(2i-1)(2j-1)} \int_0^1 \sin \frac{2i-1}{2} \pi x \sin \frac{2j-1}{2} \pi x \cos(m-1) \pi x dx \\ &= \begin{cases} -\frac{2}{\pi^2(2i-1)(2j-1)}, & i+j-1+m-1=0, \\ -\frac{2}{\pi^2(2i-1)(2j-1)}, & i-j+m-1=0, m \neq 1, \\ \frac{2}{\pi^2(2i-1)(2j-1)}, & i-j+m-1=0, m \neq 1, \\ \frac{2}{\pi^2(2i-1)(2j-1)}, & i-j-m+1=0, m \neq 1, \\ \frac{4}{\pi^2(2i-1)(2j-1)}, & i=j, m=1, \\ 0, & \text{otherwise}, \end{cases} \end{split}$$

4.2 Shifted Legendre polynomials

In order to balance the different order of trace formula, we choose polynomials $\{P_n\}_{n=1}^s$ to design a relatively stable scheme. From proposition 6 deduced in [22], we can see that for all polynomial P_n with $P_n(0) = 0$, the following equation holds:

$$\sum_{k=1}^{\infty} P_n(\lambda_k^{-1}) = \operatorname{trace} P_n(\mathbf{M}(\mathbf{a}))$$
(4.7)

In this section, we use the shifted Legendre polynomials on [0, 1] given by recursive formulae:

$$L_n(x) = \frac{2n-1}{n}(2x-1)L_{n-1}(x) - \frac{n-1}{n}L_{n-2}(x), \quad n \ge 2,$$

with

$$L_0(x) = 1, \ L_1(x) = 2x - 1.$$

Denoting $\tilde{L}_n(x) = xL_{n-1}(x)$, then we have the recursive formula

$$\tilde{L}_{n+1}(x) = \frac{2n-1}{n}(2x-1)\tilde{L}_n(x) - \frac{n-1}{n}\tilde{L}_{n-1}(x),$$

with

$$\tilde{L}_1(x) = x, \ \tilde{L}_2(x) = 2x^2 - x.$$

For evaluation of the forward map and its Jacobian, we utilize the following recursive relations:

$$\operatorname{trace}(\tilde{L}_{n+1}(\mathbf{M}(\mathbf{a}))) = \operatorname{trace}\left(\frac{2n-1}{n}(2\mathbf{M}(\mathbf{a})-1)\tilde{L}_n(x)\right) - \operatorname{trace}\left(\frac{n-1}{n}\tilde{L}_{n-1}(x)\right),$$

and

$$\frac{\partial \operatorname{trace}(\tilde{L}_{n+1}(\mathbf{M}(\mathbf{a})))}{\partial a_m} = \operatorname{trace}\left(\frac{\partial \tilde{L}_{n+1}(\mathbf{M}(\mathbf{a}))}{\partial a_m}\right)$$
$$= \operatorname{trace}\left(\frac{4n-2}{n}\frac{\partial \mathbf{M}(\mathbf{a})}{\partial a_m}\tilde{L}_n(x) + \frac{2n-1}{n}(2\mathbf{M}(\mathbf{a})-1)\frac{\partial \tilde{L}_n(\mathbf{M}(\mathbf{a}))}{\partial a_m}\right)$$
$$-\operatorname{trace}\left(\frac{n-1}{n}\frac{\partial \tilde{L}_{n-1}(\mathbf{M}(\mathbf{a}))}{\partial a_m}\right).$$

Notice

$$\frac{\partial \mathbf{M}(\mathbf{a})}{\partial a_m} = \mathbf{M}(\mathbf{e}_m).$$

4.3 Line search Newton-like method

If T_1 is slightly smaller than $\lambda_{1,1}$ and T_2 slightly smaller than $\lambda_{2,1}$, we use two uniform partitions for $[0,T_1]$ and $[0,T_2]$, i.e., $0 = t_1 < t_2 < \cdots < t_{N_1} = T_1$ and $0 = \iota_1 < \iota_2 < \cdots < \iota_{N_2} = T_2$. For every t_i , $i = 1, 2, \ldots, N_1$ and ι_i , $i = 1, 2, \ldots, N_2$, we apply them to rescale $\lambda_{1,k}$ and $\lambda_{2,k}$ respectively. With the technique of trigonometric polynomial approximation and the operator of Legendre polynomials, the inverse problem of recovering ρ comes down to solving a system of nonlinear equations with the unknown 2*M*-vector $\mathbf{a} = \{a_1, a_2, \cdots, a_{2M}\}$, i.e.,

$$F(\mathbf{a}) = \begin{pmatrix} r_{1}^{(1)}(\mathbf{a}) \\ \vdots \\ r_{N_{1}}^{(1)}(\mathbf{a}) \\ r_{1}^{(2)}(\mathbf{a}) \\ \vdots \\ r_{N_{2}}^{(2)}(\mathbf{a}) \end{pmatrix} = \begin{pmatrix} \operatorname{trace}(\tilde{L}_{s_{1}}(t_{1}\mathbf{M}^{(1)}(\mathbf{a}))) - \sum_{k=1}^{\infty} \tilde{L}_{s_{1}}(t_{1}\lambda_{1,k}^{-1}(\rho, a, b)) \\ \vdots \\ \operatorname{trace}(\tilde{L}_{s_{1}}(t_{N_{1}}\mathbf{M}^{(1)}(\mathbf{a}))) - \sum_{k=1}^{\infty} \tilde{L}_{s_{1}}(t_{N_{1}}\lambda_{1,k}^{-1}(\rho, a, b)) \\ \operatorname{trace}(\tilde{L}_{s_{2}}(\iota_{1}\mathbf{M}^{(2)}(\mathbf{a}))) - \sum_{k=1}^{\infty} \tilde{L}_{s_{2}}(\iota_{1}\lambda_{2,k}^{-1}(\rho, a, b)) \\ \vdots \\ \operatorname{trace}(\tilde{L}_{s_{2}}(\iota_{N_{2}}\mathbf{M}^{(2)}(\mathbf{a}))) - \sum_{k=1}^{\infty} \tilde{L}_{s_{1}}(\iota_{N_{2}}\lambda_{2,k}^{-1}(\rho, a, b)) \end{pmatrix} = \mathbf{0}, \quad (4.8)$$

where s_1 and s_2 are the chosen highest degree of shifted legendre polynomials. To make sure the above equations system has a unique solution, we set $N_1 + N_2 >> 2M$.

Throughout this paper we make the assumption that the vector function F is continuously differentiable in the region \mathcal{D} containing the value of **a** we are interested in. In other words, the Jacobian $J(\mathbf{a})$ defined by

$$J(\mathbf{a}) = \nabla F(\mathbf{a})^T = \begin{pmatrix} \nabla r_1^{(1)}(\mathbf{a})^T \\ \vdots \\ \nabla r_{N_1}^{(1)}(\mathbf{a})^T \\ \nabla r_1^{(2)}(\mathbf{a})^T \\ \vdots \\ \nabla r_{N_2}^{(2)}(\mathbf{a})^T \end{pmatrix},$$
(4.9)

exists and is continuous. In order to solve the above system (4.8), we apply the line search Newton-like method as

$$\mathbf{a}_{k+1} = \mathbf{a}_k + \alpha_k p_k, \ k = 0, 1, 2, \dots,$$
 (4.10)

where the Newton step p_k satisfies that

$$J(\mathbf{a}_k)p_k = -F(\mathbf{a}_k),\tag{4.11}$$

and the step length factor α_k satisfies the Wolfe conditions, i.e.,

$$\begin{cases} F(\mathbf{a}_k + \alpha_k p_k) \le F(\mathbf{a}_k) + c_1 \alpha_k J(\mathbf{a}_k) p_k, \\ J(\mathbf{a}_k + \alpha_k p_k) \ge c_2 J(\mathbf{a}_k) p_k, \end{cases}$$
(4.12)

with $0 < c_1 < c_2 < 1$.

Since systems of nonlinear equations often contain singular points, this behavior gives cause for concern. To prevent this undesirable behavior, we may have to modify the Newton direction. One possibility is to add some multiple $\sigma_k I$ of the identity to $J_k^T J_k$, and define the step p_k to be

$$p_k = -(J_k^T J_k + \sigma_k I)^{-1} J_k^T F_k.$$
(4.13)

For any $\sigma_k > 0$ the matrix in parentheses is nonsingular. Therefore, some practical algorithms choose σ_k adaptively to ensure that the matrix in (4.13) does not approach singularity. In addition, more detailed computation procedure can be referred to Algorithm 2 in Appendix.

5 Numerical simulations

In this section, we choose four kinds of examples to study the reconstruction behaviours from the first L eigenvalues of the two spectra, respectively. The reference eigenvalues used have been computed by applying the Numerov's method discussed in Section 2. For the sensitive analysis, the perturbed eigenvalues λ_i^{δ} are defined by

$$\lambda_i^{\delta} = \lambda_i + \delta \lambda_i \cdot (rand(size(\lambda_i))), \ i = 1, 2,$$

where δ is the noise level and $\lambda_i = \{\lambda_{i,1}, \lambda_{i,2}, \dots, \lambda_{i,L}\}$. As the matrix $\mathbf{M}(\mathbf{a})$ is infinite-dimensional, we shall truncate it to a $J \times J$ matrix in our computation procedure.

Example 1 We first test the density

$$\rho_1(x) = 0.98 - 0.04 \cos \pi x - 0.03 \cos 2\pi x + 0.26 \cos 3\pi x + 0.07 \cos 4\pi x - 0.04 \cos 5\pi x,$$

which is a linear combination of Fourier cosine functions with M = 3.

For numerical implementation, T_1 and T_2 should not be greater than the minimum eigenvalue corresponding to DDBCs and the minimum eigenvalue corresponding to DNBCs respectively. Besides, the size

J usually equals to the value L. Most parameters are set in Table 1. We fix the noise level $\delta = 0.5\%$. The reconstructed behaviours with different number of eigenvalues L are shown in Figure 1. As we can see from Figure 1, the inversion algorithm is effective for the reconstruction of ρ_1 . Moreover, the greater L becomes, the better ρ_1 is reconstructed.

Table 1: The settings of parameters.

h	s_1	s_2	T_1	T_2	N_1	N_2
0.004	45	60	8	2	180	180



Figure 1: These plots demonstrate the numerical recovery of ρ_1 with diffrent number of eigenvalues when noise level $\delta = 0.5\%$.

Example 2 In this second example, we consider a general continuous density

$$\rho_2(x) = 1 + (x - \frac{2}{3})^2.$$

Most parameters are also listed in Table 1. In addition, we set J = L = 20, $\delta = 0.5\%$. Figure 2 shows the reconstruction with diverse Fourier cosine functions.

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Figure 2: Figure 2(a),(c),(e) describe the reconstruction with different M and Figure 2(b)(d)(f) depict the numerical errors of recovery corresponding to their left subfigure where all the horizon lines represent the variable x.

Example 3 We next recover a non-smooth continuous function

$$\rho_3(x) = \frac{4}{5} + \frac{1}{2} \left| x - \frac{1}{3} \right|$$

in the case of J = 10 and J = 20. Fixing $s_1 = 50$, $s_2 = 70$, $T_1 = 8$, $T_2 = 2$, $N_1 = 5s_1$, $N_2 = 4s_2$, h = 0.004, $\delta = 0.5\%$, Numerical reconstructions are shown in Figure 3.



Figure 3: These two plots exhibite the recovering of $\rho_3(x)$ with M = 4.

Example 4 For the last example, the unknown denstiy is a discontinuous function

$$\rho_4(x) = \begin{cases} 0.9, & 0 \le x \le 0.3, \\ 1.1, & 0.3 < x \le 0.7, \\ 1, & 0.7 < X \le 1. \end{cases}$$

Setting $s_1 = 50$, $s_2 = 70$, $T_1 = 8$, $T_2 = 2$, $N_1 = 5s_1$, $N_2 = 4s_2$, h = 0.004, $\delta = 0.5\%$, we investigate the reconstructed behaviors with M = 5 and M = 7 which are domenstrated in Figure 4.



(a) recovery with M = 5 (b) recovery with M = 7Figure 4: These two plots show the reconstruction of ρ_4 with L = J = 20.

density	noise level $(\%)$	norm of error	density	noise level $(\%)$	norm of error
ρ_1	0	0.0005	ρ_2	0	0.0696
	0.1	0.0012		0.1	0.0835
	0.5	0.0083		0.5	0.0954
	1	0.0254		1	0.1167
ρ_3	0	0.0178	$ ho_4$	0	0.1017
	0.1	0.0233		0.1	0.1034
	0.5	0.0300		0.5	0.1180
	1	0.0514		1	0.2773

Table 2: Inversion errors of non-symmetric density functions in using the maximum norm.

Through Figure 1-3, one can clearly observe that the reconstructed non-symmetric density functions are in good agreement with their true solutions. Compared with the three mentioned densities, the reconstruction for discontinuous function ρ_4 shown in Figure 4 is the worst, but even in this case the recovered function still resembles its exact solution. For sensitive analysis, Table 2 illustrates the results of inversion algorithm to recover these four kinds of densities where noisy eigenvalues are provided with noise levels of 0.1%, 0.5%, 1%, respectively. One can see that our proposed reconstruction method stays stable.

6 Conclusions and Acknowledgments

In this paper, we introduce a new method to solve the inverse Sturm-Liouville problem in the nonsymmetric case. It is based on the Lidskii's theorem and Mercer's theorem. A series of trace fomulas that combining the eigenvalues and the density in (1.1) are built by the two theorems. In our computation procedure, therefore, we only need to compute eigenvalues once that is totally different from the previous methods introduced in [1, 3–5, 9, 13, 14]. Furthermore, our work provides a new possibility for solving inverse higher order Sturm-Liouville problem. This work was partially supported by NSFC 11621101, 91630309 and the Fundamental Research Funds for the Central Universities.

Appendix. Detailed algorithm for inverse problem

Algorithm 1 Calculating Jacobian and traces with Legendre polynomials **Input:** $a = (a_1, a_2, ..., 2M), M(a), s;$ Output: $J(\mathbf{a})$, trace $(\tilde{L}_s(\mathbf{M}(\mathbf{a})))$; 1: Compute $\tilde{L}_2(\mathbf{M}(\mathbf{a})), \frac{\partial \tilde{L}_2(\mathbf{M}(\mathbf{a}))}{\partial a_m};$ 2: $d_1 = \operatorname{trace}(\mathbf{M}(\mathbf{a}));$ 3: $d_2 = \operatorname{trace}(\tilde{L}_2\mathbf{M}(\mathbf{a}));$ 4: for $1 \leq m \leq 2M$ do $J_{1,m} = \operatorname{trace}(\mathbf{M}(\mathbf{a}));$ 5: $J_{2,m} = \operatorname{trace}\left(\frac{\partial \mathbf{M}(\mathbf{a})}{\partial a_m}\right);$ 6: 7: end for 8: for $2 \le i \le s - 1$ do $\tilde{L}_{i+1}(\mathbf{M}(\mathbf{a})) = \frac{2i-1}{i}(2\mathbf{M}(\mathbf{a}) - 1)\tilde{L}_i(x) - \frac{i-1}{i}\tilde{L}_{i-1}(x);$ 9: 10: for $1 \leq m \leq 2M$ do $\frac{\partial \tilde{L}_{i+1} \mathbf{M}(\mathbf{a})}{\partial a_m} = \left(\frac{4i-2}{i} \mathbf{M}(\mathbf{e}_m)\right) \tilde{L}_i(x) + \frac{2i-1}{i} (2\mathbf{M}(\mathbf{a})-1) \frac{\partial \tilde{L}_i(\mathbf{M}(\mathbf{a}))}{\partial a_m} - \frac{i-1}{i} \frac{\partial \tilde{L}_{i-1}(\mathbf{M}(\mathbf{a}))}{\partial a_m};$ 11: 12:end for $d_{i+1} = \operatorname{trace}(\tilde{L}_{i+1}(\mathbf{M}(\mathbf{a})));$ 13:for $2 \leq i \leq s - 1$ do 14: $J_{i+1,m} = \operatorname{trace}\left(\frac{\partial \tilde{L}_{i+1}(\mathbf{a})}{\partial a_m}\right);$ 15:end for 16:17: end for

Algorithm 2 Inversion of trace formulae with line search Newton-like method

1: Given maximum number iteration N;

2: Given c_1, c_2 with $0 < c_1 < c_2 < \frac{1}{2}$ and regularized parameter σ ;

- 3: Choose initial value \mathbf{a}_0 ;
- 4: Caculate the first N_1 eigenvalues $\lambda_{1,1}, \lambda_{1,2}, \ldots, \lambda_{1,N_1}$ as well as the first N_2 eigenvalues $\lambda_{2,1}, \lambda_{2,2}, \ldots, \lambda_{2,N_2}$;
- 5: Compute $\mathbf{M}^{(1)}(\mathbf{e}_m), \ \mathbf{M}^{(2)}(\mathbf{e}_m);$

6: Compute
$$\gamma^{true} = \left(\sum_{k=1}^{\infty} \tilde{L}_{s_1}(t_1\lambda_{1,k}^{-1}), \cdots, \sum_{k=1}^{\infty} \tilde{L}_{s_1}(t_{N_1}\lambda_{1,k}^{-1}), \sum_{k=1}^{\infty} \tilde{L}_{s_2}(\iota_1\lambda_{2,k}^{-1}), \cdots, \sum_{k=1}^{\infty} \tilde{L}_{s_2}(\iota_{N_2}\lambda_{2,k}^{-1})\right);$$

7: for $1 \le k \le N$ do

- 8: Caculate $J^{(1)}(\mathbf{a}_{k-1})$ and $\gamma^{(1)} = \left(\operatorname{trace}(\tilde{L}_{s_1}(t_1 \mathbf{M}^{(1)}(\mathbf{a}_{k-1}))), \cdots, \operatorname{trace}(\tilde{L}_{s_1}(t_{N_1} \mathbf{M}^{(1)}(\mathbf{a}_{k-1}))) \right)$ with $\mathbf{M}^{(1)}(\mathbf{e}_m)$ through Algorithm 1;
- 9: Caculate $J^{(2)}(\mathbf{a}_{k-1})$ and $\gamma^{(2)} = \left(\operatorname{trace}(\tilde{L}_{s_1}(\iota_1 \mathbf{M}^{(2)}(\mathbf{a}_{k-1}))), \cdots, \operatorname{trace}(\tilde{L}_{s_1}(\iota_{N_1} \mathbf{M}^{(2)}(\mathbf{a}_{k-1}))) \right)$ with $\mathbf{M}^{(2)}(\mathbf{e}_m)$ through Algorithm 1;
- 10: $J(\mathbf{a}_{k-1}) = (J^{(1)}; J^{(2)});$
- 11: $\gamma = (\gamma^{(1)}; \gamma^{(2)});$
- 12: $F(\mathbf{a}_{k-1}) = \gamma \gamma^{ture};$
- 13: Calculate p_{k-1} by the equation (4.13);
- 14: **if** $\alpha = 1$ satisfies the Wolfe conditions (4.12) **then**
- 15: Set $\alpha_{k-1} = 1;$
- 16: else
- 17: Perform a line search to find $\alpha_{k-1} > 0$ that satisfies (4.12)
- 18: end if

19: $\mathbf{a}_k = \mathbf{a}_{k-1} + \alpha_{k-1} p_{k-1};$ 20: end for

References

- L. Aceto, P. Ghelardoni, C. Magherini, Boundary value methods for the reconstruction of Sturm-Liouville potentials, Appl. Math. Comput. 219(2012) 2960-2974.
- [2] A. L. Andrew, Numerov's method for inverse Sturm-Liouville problem, Inverse Probl. 21(2005). 223-238.
- [3] A.L. Andrew, Finite difference methods for half inverse Sturm-Liouville problem, Appl. Math. Comput. 218(2011) 445-457.
- [4] A.L. Andrew, Computing Sturm-Liouville potentials from two spectra. Inverse Probl. 22 (2006) 2069-2081.
- [5] C. Böckmann, A. Kammanee, Broyden method for inverse non-symmetric Sturm-Liouville problems, BIT Numer Math 51(2011) 513-528.
- [6] C. Borg, Eine umkehrug der Sturm-Liouvilleschen eigenwertaufgabe, Acta Math. 78(1946) 732-53.
- [7] R. H. Fabiano, R. Knoel, B. D. Lowe, A finite-difference algorithm for an inverse Sturm-Liouville problem, J. Numer. Anal. 15(1995) 75-88.
- [8] Q. Gao, X. Cheng, Z. Huang, On a boundary value method for computing Sturm-Liouville potentials from two spectra, International J. Comp. Math. 91(3)) (2014) 490-513.
- [9] P. Ghelardoni, C. Magherini, BVMs for computing Sturm-Liouville symmetrc potentials, Appl. Math. Comput. 217(2010) 3032-3045.
- P. Ghelardoni, Approximations of Sturm-Liouville eigenvalues using boundary value methods. Appl. Numer. Math. 23 (1997) 311-325.
- [11] J. C. Gilbert, On the realization of the Wolf conditions in reduced Quasi-Newton for equality constrained optimization, SIAM J. Optim. 7(3) (1997) 780-813.
- [12] L. Grippo, F. Lampariello, S. Lucidi, A nonmonotone line search technique for Newton's method, SIAM J. Numer. Anal. 23(4) (1986) 707-716,
- [13] A. Kammanee, C. Böckmann, Boundary value method for inverse Sturm-Liouville problems, Appl. Math. Comput, 214(2009) 342-352.
- [14] A. Kammanee, C. Böckmann, Determination of partially known Sturm-Liouville potentials, Appl. Math. Comput. 204(2008) 928-937.
- [15] J. D. Pryce, Numerical solution of Sturm-Liouville problems, Oxford University, New York, 1993.
- [16] N. Röhrl, A least-squares functional for solving inverse Sturm-Liouville problems, Inverse Probl. 21(2005) 2009-2017.
- [17] W. Rundell, P.E. Sacks, Reconstruction techniques for classical inverse Sturm-Liouville problems, Math. Comp. 58(197) (1992) 161-183.
- [18] P.E. Sacks (2015) Inverse Spectral Problems: 1-D, Algorithms. In: Engquist B. (eds) Encyclopedia of Applied and Computational Mathematics. Springer, Berlin, Heidelberg.
- [19] C. L. Shen, On the Liouville transformation and some inverse spectral problems, Inverse Probl. 21(2005) 591-619.
- [20] C. L. Shen, The Liouville transformation, the density function, and the complete transformability problem of the potential equation, Inverse Probl. 21(2005) 615-34.
- [21] M. Sini (2015) Inverse Spectral Problems: 1-D, Theoretical Results. In: Engquist B. (eds) Encyclopedia of Applied and Computational Mathematics. Springer, Berlin, Heidelberg.
- [22] X. Xu, J. Zhai, Inverseion of trace formulae for a Sturm-Liouville operator, 2019. arXiv:1906.12108v1.
- [23] H. Zhang, W. Hager, A nonmonotone line search technique and its application to unconstrained optimization, SIAM J. Optim. 14(4) (2004) 1043-1056.