INVERSE STURM-LIOUVILLE SYSTEMS OVER THE WHOLE REAL LINE

A THESIS SUBMITTED TO
THE GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES
OF
MIDDLE EAST TECHNICAL UNIVERSITY

BY

HÜSEYİN ALTUNDAĞ

IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR
THE DEGREE OF DOCTOR OF PHILOSOPHY
IN
MATHEMATICS

NOVEMBER 2010

Approval of the thesis:

INVERSE STURM-LIOUVILLE SYSTEMS OVER THE WHOLE REAL LINE

submitted by **HÜSEYİN ALTUNDAĞ** in partial fulfillment of the requirements for the degree of **Doctor of Philosophy in Mathematics Department, Middle East Technical University** by,

Prof. Dr. Canan Özgen _____
Dean, Graduate School of **Natural and Applied Sciences**

Prof. Dr. Zafer Nurlu _____
Head of Department, **Mathematics**

Prof. Dr. Hasan Taşeli _____
Supervisor, **Mathematics, METU**

Examining Committee Members:

Prof. Dr. Marat U. Akhmet
Mathematics Dept., METU _____

Prof. Dr. Hasan Taşeli
Mathematics Dept., METU _____

Prof. Dr. Tanıl Ergenç
Mathematics Dept., Atılım Univ. _____

Assoc. Prof. Dr. Hakan I. Tarman
Engineering Science Dept., METU _____

Assoc. Prof. Dr. Ömür Uğur
Institute of Applied Mathematics., METU _____

Date: _____

I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all material and results that are not original to this work.

Name, Last Name: HÜSEYİN ALTUNDAĞ

Signature :

ABSTRACT

INVERSE STURM-LIOUVILLE SYSTEMS OVER THE WHOLE REAL LINE

Altundağ, Hüseyin
Ph. D., Department of Mathematics
Supervisor: Prof. Dr. Hasan Taşeli

November 2010, 88 pages

In this thesis we present a numerical algorithm to solve the singular Inverse Sturm-Liouville problems with symmetric potential functions. The singularity, which comes from the unbounded domain of the problem, is treated by considering the limiting case of the associated problem on the symmetric finite interval. In contrast to regular problems which are considered on a finite interval the singular inverse problem has an ill-conditioned structure despite of the limiting treatment. We use the regularization techniques to overcome the ill-posedness difficulty. Moreover, since the problem is nonlinear the iterative solution procedures are needed. Direct computation of the eigenvalues in iterative solution is handled via psoudespectral methods. The numerical examples of the considered problem are given to illustrate the accuracy and convergence behaviour.

Keywords: Singular inverse Sturm-Liouville systems, ill-posed equations, regularization, pseudospectral method.

ÖZ

REEL EKSEN ÜZERİNDE TANIMLANMIŞ TERS STURM-LIOUVİLLE SİSTEMLERİ

Altundağ, Hüseyin
Doktora, Matematik Bölümü
Tez Yöneticisi: Prof. Dr. Hasan Taşeli

Kasım 2010, 88 sayfa

Bu çalışmada tekil özelliğe sahip olan ters Sturm-Liouville probleminde simetrik potansiyel fonksiyonları için sayısal algoritma üretildi. Problemin sonsuz aralık üzerinde tanımlanmış olmasından kaynaklanan tekillik, sonsuz aralığa karşılık gelen sonlu simetrik aralık üzerinde giderilmeye çalışıldı. Ancak sonlu aralıkta tanımlanan tekil olmayan ters problemin aksine, tekil problemin, sonlu aralığa indirgenmiş olmasına rağmen hastalıklı (ill-posed) bir yapısının olduğu görüldü. Bu yapıyı düzeltmek için iyileştirme (regularization) teknikleri kullanıldı. Ayrıca sayısal anlamda çözümü aranan problemin doğrusal olmamasından dolayı özyinelemeli metod kullanıldı. Bu metodta ihtiyaç duyulan düz problemin çözümü sankispektral metodlar yardımıyla elde edildi. Doğruluğun ve yakınsaklığın sergilenmesi amacıyla varsayılan problem için sayısal örnekler verildi.

Anahtar Kelimeler: Tekil Sturm-Liouville problemleri, hastalıklı denklemler, iyileştirme, sanki-spektral metodlar.

To owners of my heart: Pınar and Çınar

ACKNOWLEDGMENTS

I would like to express my sincere gratitude to my supervisor, Prof. Dr. Hasan Taşeli for his support, guidance and encouragement throughout the research. It has been a pleasure to have worked with him.

I offer a special thank to Dr. Christine Böckmann for her guidance and encouragement, providing a good environment and facilities in my research throughout my visit Potsdam, Germany.

Many thanks also go to Haydar Alıcı and Rezan Sevinik for their valuable friendships and ideas helping me.

I deeply thank all the members of the Department of Mathematics of METU for the atmosphere they provided that broadened my horizons during my graduate work. I am also grateful to all my friends in University of Potsdam.

I will also never forget the unending support, encouragement and love my family has provided me all my life.

Last, but not the least I owe my deepest gratitude to my wife Pınar Altundağ for her endless love and supporting me spiritually throughout our life.

This research has been supported by a grant from Tübitak, the Scientific and Technical Research Council of Turkey.

TABLE OF CONTENTS

LIST OF TABLES

TABLES

LIST OF FIGURES

FIGURES

CHAPTER 1

INTRODUCTION

1.1 Introductory Background

Differential equations are of interest for both pure and applied mathematicians. While pure mathematicians study on the existence and uniqueness of solutions, applied mathematicians are more interested in dealing with practical computational procedures of differential equations. In this dissertation we focused on the numerical solution of the inverse Sturm-Liouville problems. At the beginning of the thesis we mention briefly about definitions, notations and theorems that will be used later on.

Definition 1.1 *(Normed, Banach and Hilbert Spaces, Inner Product Space) Let X be a vector space over a field of scalars $\mathbb{F}$. We assume that there exists a real-valued non-negative function $\|.\| : X \to \mathbb{R}^+$ satisfying*

(i) $\|x\| \geq 0$ *for all* $x \in X$ *and* $\|x\| = 0$ *iff* $x = 0$

(ii) $\|\alpha x\| = |\alpha|\|x\|$ *for all* $x \in X$, $\alpha \in \mathbb{F}$

(iii) $\|x + y\| \leq \|x\| + \|y\|$ *for all* $x, y \in X$.

Such a function is called norm on X and a vector space X with this norm is said to be normed space denoted by $(X, \|.\|)$. Given a normed space, define $d(x, y) = \|x - y\|$ for all $x, y \in X$. Then d is a metric for X induced by the norm $\|x\|$.

A sequence (x_n) is said to be a Cauchy sequence in X equipped with a norm if $\|x_n - x_m\| \to 0$ as $m, n \to \infty$. A sequence (x_n) in X is said to converge to a vector x in X if $\|x_n - x\| \to 0$ as $n \to \infty$.

A vector space X is complete if every Cauchy sequence in X converges to an element of X. A normed space which is complete in the metric defined by its norm is called a Banach space.

Now, let X be a vector space over complex numbers $\mathbb{C}$. An inner product on X is a function $\langle , \rangle : X \times X \to \mathbb{C}$ which satisfies the following axioms:

(i) $\langle x, y\rangle = \overline{\langle y, x\rangle}$

(ii) $\langle \alpha x, y\rangle = \alpha \langle x, y\rangle$

(iii) $\langle x + y, z\rangle = \langle x, z\rangle + \langle y, z\rangle$

(iii) $\langle x, x\rangle \geq 0$ *and* $\langle x, x\rangle = 0$ *iff* $x = 0$.

An overbar denotes the complex conjuge and $x, y, z \in X$, $\alpha \in \mathbb{C}$. A vector space endowed with an inner product is called an inner product space. Every inner product space is a normed space with a natural norm $\|x\| = \langle x, x\rangle^{1/2}$.

A Hilbert space is a complete inner product space, i.e., is a Banach space whose norm is defined by an inner product.

Definition 1.2 *(Linear, Bounded, Adjoint Operator) Let X and Y be vector spaces over a field $\mathbb{F}$. A linear operator T of X into Y is an operator $T : X \to Y$ such that $T(\alpha x + \beta y) = \alpha T(x) + \beta T(y)$ for all $x, y \in X$, $\alpha, \beta \in \mathbb{F}$.*

T is a bounded operator if X, Y are normed vector spaces and $\|Tx\| \leq c\|x\|$ holds for $c \in \mathbb{F}$. Moreover, the smallest c satisfying the inequality is called the norm of the operator T denoted by $\|T\|$.

Let X, Y be Hilbert spaces and $T : X \to Y$ be a linear operator. An operator $T^* : Y \to X$ is called the adjoint operator of T if $\langle Tx, y\rangle = \langle x, T^*y\rangle$ for all $x \in X$ and $y \in Y$. If the relation $Tx = T^*x$ is satisfied for all $x \in X$, then operator T is said to be self-adjoint.

Definition 1.3 *Let X be an inner product space and x, y be vectors in X. If $\langle x, y\rangle = 0$ then x and y are said to be orthogonal. Now let U be a non-empty subset of X then*

the set $U^{\perp} = \{x \in X : \langle x, u\rangle = 0 \ \text{for all } u \in U\}$ *is called the orthogonal complement of* U.

Definition 1.4 *(Orthonormal Basis) Let* $E = \{e_i\}$ *be a non-empty subset of a Hilbert space H. If* $(i)\ e_i \perp e_j$ *if* $i \neq j$, $(ii)\ \|e_i\| = 1\ \forall i$
then the set E *is called an orthonormal set of H. In other words an orthonormal set in a Hilbert space H is a non-empty subset of H which consist of mutually orthogonal unit vectors. An orthonormal set* E *in an inner product space H is called complete if it is not possible to add a non-zero vector e to a set* $E = \{e_i\}$ *such that the enlarged set* $\{e_i, e\}$ *turns out to be orthonormal. A complete orthonormal set in a Hilbert space is called an orthonormal basis or Hilbert basis.*

Theorem 1.5 *Let E be a orthonormal set of a Hilbert space H. Then the followings are equivalent:*

(a) E *is complete*

(b) If $\langle u, e\rangle = 0$ *for all* $e \in E$, *then* $u = 0$

(c) $u = \sum_{e_i \in E} \langle u, e_i\rangle\, e_i$ *for all* $u \in H$

(d) $\|u\|^2 = \sum_{e_i \in E} |\langle u, e_i\rangle|^2$ *for all* $u \in H$.

For a proof see [72]. The series in (c) is known as Fourier series and the coefficients $\langle u, e_i\rangle$, $i = 1, 2, \ldots$ are called Fourier coefficients. The identity in (d) is called Parseval identity.

Definition 1.6 *(The Resolvent Set and The Spectrum of an Operator) Let* T *be a linear operator on a normed space* X. *The set* $\varrho(T) \in \mathbb{C}$ *of all complex numbers* λ *for which the operator* $T_\lambda = \lambda I - T$ *has a dense range* $\mathcal{R}_\lambda = \mathcal{R}(T_\lambda)$ *in* X *and* T_λ *has a continuous inverse is called the resolvent set of the operator* T. *The complement of this set in* $\mathbb{C}$, *namely* $\sigma(T) = \mathbb{C} - \varrho(T)$ *is called the spectrum of the operator* T. *Moreover, if* $\lambda \in \sigma(T)$, *then either* ${T_\lambda}^{-1}$ *does not exist; or* ${T_\lambda}^{-1}$ *exist, but it is not continuous; or* ${T_\lambda}^{-1}$ *exist, but* $\overline{\mathcal{R}_\lambda} \neq X$. *We should note that the domain of* ${T_\lambda}^{-1}$ *is*

equal to the range of T_λ, i.e., $\mathcal{D}(T_\lambda{}^{-1}) = \mathcal{R}_\lambda$ if T_λ has an inverse. Thus, the spectrum can be decomposed into three disjoint sets as follows:

1. *The set $\sigma_p(T) = \left\{\lambda \in \mathbb{C}; T_\lambda{}^{-1}\text{does not exist}\right\}$ which is known as point spectrum of T and its members are called eigenvalues of T. For the elements of the spectrum there are non-zero vectors from X such that $Tx = \lambda x$ satisfied. These vectors are known as eigenvectors of T and constitute a subspace $W(\lambda) \subseteq X$ which is called the characteristic subspace associated with λ. The dimension of this subspace, which maybe infinite, is the multiplicity of the eigenvalue λ.*
2. *The set $\sigma_c(T) = \left\{\lambda \in \mathbb{C}; T_\lambda{}^{-1}\text{ exist but it is unbounded}\right\}$ is called the continuous spectrum of T.*
3. *The set $\sigma_r(T) = \left\{\lambda \in \mathbb{C}; T_\lambda{}^{-1}\text{ exist but } \overline{\mathcal{R}_\lambda} \neq X\right\}$ is called the residual spectrum of T.*

These decompositions lead evidently $\sigma(T) = \sigma_p(T) + \sigma_c(T) + \sigma_r(T)$.

Remark 1.7 *A linear operator on a finite dimensional vector space might have only the point spectrum.*

Definition 1.8 *Assume that ϵ_0 represents an initial error and ϵ_n represents the growth of the error after n steps. If $|\epsilon_n| \sim n\epsilon_0$, the growth of error is said to be linear. If $|\epsilon_n| \sim \epsilon_0 K^n$ the growth of the error is called exponential. In this case, if $K > 1$ the exponential error grows without bound as $n \to \infty$, and if $K < 1$ the exponential error vanishes as $n \to \infty$.*

Definition 1.9 *(Fréchet Derivative of an Operator) Let T be a mapping between a Banach space X and a Banach space Y, i.e., $T : X \to Y$. We say that T is Fréchet differentiable at a point $u_0 \in X$ if there exist a linear continuous operator L from X to Y such that*

$$\lim_{w \in X,\, \|w\|_X \to 0} \frac{\|T(u_0 + w) - T(u_0) - Lw\|_Y}{\|w\|_X} = 0.$$

If this happens, the linear operator L is unique. It is termed the Fréchet derivative of T at the point u_0.

Remark 1.10 *Fréchet derivative represents the usual derivative if T is defined between finite dimensional spaces. Thus, the existence of the Jacobian matrix guarantees the Fréchet differentiability condition for nonlinear equation systems.*

1.2 Sturm Liouville Theory

1.2.1 Sturm Liouville Problem

Second order linear differential equations are frequently encountered in practice in connection with physical and engineering problems. One of the most famous problem is the Sturm-Liouville eigenvalue problem

$$Ly(x) = 0\,, \quad x \in (a,b) \tag{1.1}$$

with the formally self-adjoint operator L defined by

$$L = -\frac{\mathrm{d}}{\mathrm{d}x}\Big[p(x)\frac{\mathrm{d}}{\mathrm{d}x}\Big] + q(x) - \lambda r(x) \tag{1.2}$$

where $p(x)$ and $r(x)$ are strictly positive, $p(x), q(x)$ and $r(x)$ are assumed to be real-valued continuous functions except for finitely many jumps on the interval (a,b) and λ is a real parameter. The boundary conditions accompanying with (1.1) will be

$$\begin{aligned} y(a)\cos(\alpha) + y'(a)\sin(\alpha) &= 0 \\ y(b)\cos(\beta) + y'(b)\sin(\beta) &= 0 \end{aligned} \tag{1.3}$$

where α and β are real numbers between 0 and π. If a and b are finite, the system consisting of (1.1)-(1.3) is called regular Sturm-Liouville system. The parameter λ for which the equation (1.1) has nontrivial solution subject to boundary conditions (1.3) is called eigenvalue and the corresponding nontrivial solution $y(x)$ is called eigenfunction of the system.

For example, in quantum mechanics one dimensional motion of a particle of mass m in an external field V is represented by the equation

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x)$$

in which $\psi(x)$ is the wave function, E is the total energy of the particle and $\hbar$ is the Planck constant divided by 2π. This equation is called Schrödinger equation which is a special form of a Sturm-Liouville problem.

If we deal with the vibrational modes of a string, sound waves in a pipe or certain mechanical systems, we reach the time dependent wave equation

$$\frac{\partial}{\partial x}\Big[p(x)\frac{\partial u}{\partial x}\Big] - q(x)u = r(x)\frac{\partial^2 u}{\partial t^2}$$

where $p(x)$ is denoted by tension of the string, $q(x)$ is spring-like transverse restoring force, and $r(x)$ is the density of the string. When we propose separation of variables of the form $u(x,t) = \phi(x)sin(\omega t)$ then $\phi(x)$ must satisfy

$$\frac{\mathrm{d}}{\mathrm{d}x}\Big[p(x)\frac{\mathrm{d}\phi}{\mathrm{d}x}\Big] - q(x)\phi = \lambda r(x)\phi$$

which is the standard form of the Sturm-Liouville equation. Here we use $\lambda = \omega^2$.

It is well known that the Sturm-Liouville problem has nice mathematical properties.

Proposition 1.11 *For a regular Sturm-Liouville problem,*

(i) Eigenvalues are real, simple and they constitute an increasing sequence $\lambda_0 < \lambda_1 < \ldots$ tend to ∞.

(ii) The eigenfunctions corresponding to distinct eigenvalues are orthogonal and form a complete orthogonal set of functions over (a,b) with respect to the inner product

$$\langle u, v\rangle = \int_a^b uvwdx$$

under the weight function $w(x) > 0$.

(iii) (Interlacing property) y_k has exactly k zeros in the open interval (a,b) and there exist exactly one zero of y_k between two consecutive zeros of y_{k+1}. Here y_k be the kth eigenfunction corresponding to kth eigenvalue λ_k.

For proofs see for example [20].

However, Sturm-Liouville problems are also defined on an infinite intervals, namely $a = -\infty$ and/or $b = \infty$. It is also possible that one of the functions $p(x)$, $q(x)$, $r(x)$ in Sturm-Liouville problems fails to satisfy to be continuous or to be strictly positive at one or both endpoints. These types are classified as singular Sturm-Liouville problems.

One can solve Sturm-Liouville problems either analitically or numerically for a given set of functions $p(x), q(x), r(x)$ and corresponding boundary conditions with α and β to find eigenvalues and corresponding eigenfunctions. Such problems are called direct Sturm-Liouville problems. It is not easy to solve direct problems analytically, actually many of them it is impossible. This needs to develop many numerical methods giving eigenvalues and eigenfunctions in a desirable accuracy for either regular or singular problems. These methods can be classified into two main groups known as shooting and matrix methods. Basically, shooting methods [48, 63, 64] replace the boundary value problem (BVP) with an initial value problem (IVP) over the range $[a, b]$ and solve this IVP for trial values of λ until the boundary conditions at a and b can be satisfied at the same time. The principal of a matrix method is to convert differential equation to a matrix eigenvalue problem and solve it numerically [9, 73].

1.2.2 Transformation to the Schrödinger (Canonical) Form

Consider the singular Sturm-Liouville equation,

$$Ly = 0, \quad L = -\frac{\mathrm{d}}{\mathrm{d}t}\Big[p(t)\frac{\mathrm{d}}{\mathrm{d}t}\Big] + q(t) - \lambda r(t), \quad t \in (-\infty, \infty). \tag{1.4}$$

Let us transform, first, the dependent variable from $y(t)$ to $u(t)$, where

$$y(t) = \phi(t)u(t) \tag{1.5}$$

and $\phi(t)$ will be determined suitably. Since

$$y' = \phi' u + \phi u', \qquad y'' = \phi'' u + 2\phi' u' + \phi u''$$

we have from (1.4),

$$-\frac{\mathrm{d}^2 u}{\mathrm{d}t^2} - [2\frac{\phi''}{\phi} + \frac{p'}{p}]\frac{\mathrm{d}}{\mathrm{d}t} - [\frac{\phi''}{\phi} + \frac{p'}{p}\frac{\phi'}{\phi} - \frac{q - \lambda r}{p}]u = 0. \tag{1.6}$$

Let us now transform the independent variable from t to x by means of the substitution

$$x = f(t) \tag{1.7}$$

where f is a sufficiently smooth function. By chain rule, we have

$$\frac{\mathrm{d}u}{\mathrm{d}t} = \frac{\mathrm{d}u}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}t} \Rightarrow \frac{\mathrm{d}}{\mathrm{d}t} \equiv f'(t)\frac{\mathrm{d}}{\mathrm{d}x} \tag{1.8}$$

and

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} \equiv [f'(t)]^2 \frac{\mathrm{d}}{\mathrm{d}x^2} + f''(t)\frac{\mathrm{d}}{\mathrm{d}x} \tag{1.9}$$

where $t = f^{-1}(x)$ on the right hand side of operations in (1.8), (1.9). By means of (1.5) and (1.7), choosing $f(t)$ and $\phi(t)$ appropriately, we shall transform the original Sturm-Liouville equation into a simpler form.

From (1.8) and (1.9), we put (1.6) into the form

$$-[f'(t)]^2 \frac{\mathrm{d}^2 u}{\mathrm{d}x^2} - \left\{ f''(t) + [2\frac{\phi'(t)}{\phi(t)} + \frac{p'(t)}{p(t)}] f'(t) \right\} \frac{\mathrm{d}u}{\mathrm{d}x}$$
$$- \left\{ \frac{\phi''(t)}{\phi(t)} + \frac{p'(t)}{p(t)}\frac{\phi'(t)}{\phi(t)} - \frac{q(t)}{p(t)} + \lambda \frac{r(t)}{p(t)} \right\} u = 0.$$

with $t = f^{-1}(x)$ which can be written as

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} + F(x)\frac{\mathrm{d}u}{\mathrm{d}x} + [\lambda G(x) - V(x)] = 0 \tag{1.10}$$

where

$$F(x) = \left. \frac{2p(t)f'(t)\phi'(t) + [p(t)f'(t)]'\phi(t)}{p(t)\phi(t)[f'(t)]^2} \right|_{t=f^{-1}(x)} \tag{1.11}$$

$$G(x) = \left. \frac{r(t)}{p(t)[f'(t)]^2} \right|_{t=f^{-1}(x)} \tag{1.12}$$

$$V(x) = \left. \frac{q(t)\phi(t) - [p(t)\phi'(t)]'}{p(t)\phi(t)[f'(t)]^2} \right|_{t=f^{-1}(x)} \tag{1.13}$$

Remark 1.12 *The main idea behind our method is to consider the singular problem over a finite interval $t \in (-l, l)$, instead of $t \in (-\infty, \infty)$.*

Such a singular problem can be defined over a symmetric x-interval, $x \in (-l, l)$ if we choose

$$[f'(t)]^2 = \frac{1}{L^2}\frac{r(t)}{p(t)}, \quad L \geq 0 \tag{1.14}$$

where L will become obvious. Then,

$$f'(t) = \frac{1}{L}\sqrt{\frac{r(t)}{p(t)}} \quad \Rightarrow \quad f(t) = \frac{1}{L}\int_{-l}^{t} \sqrt{\frac{r(s)}{p(s)}}\mathrm{d}s. \tag{1.15}$$

Thus, choose L to be

$$L = \int_{-l}^{-l} \sqrt{\frac{r(s)}{p(s)}}\mathrm{d}s \tag{1.16}$$

hence the transformation in (1.7) is made explicit, i.e.,

$$x = f(t) = \frac{1}{L}\int_{-l}^{t}\sqrt{\frac{r(s)}{p(s)}}\mathrm{d}s. \tag{1.17}$$

Further, from (1.12) and (1.14), we have

$$G(x) = L^2 = \text{constant}. \tag{1.18}$$

On the other hand, $\phi(t)$ can be chosen in a way such that $F(x)$ in (1.11) vanishes. Indeed, $F(x) = 0$ if

$$2p(t)f'(t)\phi'(t) + [p(t)f'(t)]'\phi(t) = 0$$

that is

$$\frac{\phi'(t)}{\phi(t)} = -\frac{[p(t)f'(t)]'}{2p(t)f'(t)}$$

If we differentiate both side of last expression with respect to t we have,

$$\begin{aligned}\ln\left|\phi(t)\right| &= -\tfrac{1}{2}\ln\left|p(t)f'(t)\right| \\ &= -\tfrac{1}{4}\ln\left[p(t)f'(t)\right]^2 \\ &= -\tfrac{1}{4}\ln\left\{\frac{1}{L^2}p(t)r(t)\right\}\end{aligned}$$

on using (1.14). Hence we find that

$$\Phi(t) = \sqrt{L}\,[p(t)r(t)]^{-1/4}. \tag{1.19}$$

As a result equation (1.10) reduces to

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + \left[\lambda L^2 - V(x)\right]u = 0$$

or

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + [E(l) - V(x)]u = 0, \qquad x \in (-l, l). \tag{1.20}$$

Note that the new eigenvalue parameter is of the form

$$E(l) = L^2\lambda(l),$$

with L defined by (1.16).

Remark 1.13 *Such kind of transformations are known as Liouville transformations.*

Remark 1.14 *The boundary conditions accompanying with (1.20) will be*

$$u(-l)\cos(\alpha) + u'(-l)\sin(\alpha) = 0 \tag{1.21}$$

$$u(l)\cos(\beta) + u'(l)\sin(\beta) = 0 \tag{1.22}$$

in which α and β are real numbers between 0 and π. Clearly the particular values of α and β give some special type boundary conditions. For example, $\alpha = \beta = 0$ corresponds to Dirichlet, $\alpha = \beta = \frac{\pi}{2}$ corresponds to Neumann, $\alpha = 0$ and $\beta = \frac{\pi}{2}$ corresponds to mixed boundary conditions.

Remark 1.15 *If $p(t) = r(t) = 1$ in (1.4), i.e., the original equation is already in Schrödinger form.*

Remark 1.16 *The function $V(x)$ in (1.20) is called "potential function". We assume that the problem has a "reflection symmetry" under the replacement of x by $-x$. Therefore we are looking for a potential function which is even, i.e., $V(x) = V(-x)$.*

Remark 1.17 *The equation (1.20) in Schrödinger form will be considered from now on with the notation*

$$-y'' + q(x)y = \lambda y, \quad x \in (a, b) \tag{1.23}$$

for the sake of consistency with the literature.

1.2.3 What are Inverse Problems?

If information about eigenvalues and eigenfunctions are available in a Sturm-Liouville system the coefficients $p(x)$, $q(x)$, $r(x)$ can be reconstructed numerically. Problems of this kind are called inverse Sturm-Liouville problems.

A problem is called well-posed in reference to the Hadamard definition of well-posedness if the following conditions hold:

(a) A solution of the problem exists,

(b) The solution of the problem is unique,

(c) The solution is insensitive to the changes of the initial data.

Otherwise, i.e., if one of the conditions defined above is violated the problem is ill-posed. In contrast to direct problems, inverse Sturm-Liouville problems have generally ill-posed structure and cause some numerical difficulties. One of the most effective way to overcome ill-posedness is the regularization. In this thesis we shall use regularization techniques to solve singular inverse Sturm-Liouville (S-L) problems on the real line. There are several methods to solve inverse problems on a finite interval and most of them do not require regularization techniques. Singular inverse S-L problems with singularity at endpoints can be considered on the truncated domain. Since this treatment does not make it a regular one it still needs regularization. We present numerical results in Chapter 4 for singular S-L problems over $(-\infty, \infty)$ for the symmetric potential $q(x)$ if the spectrum, i.e., the eigenvalue set, is known.

1.2.4 Literature Review for Inverse Sturm-Liouville Problem

The development of the inverse spectral theory of the Sturm-Liouville equations has a long history. The starting point of the problem is the paper published in 1929 by Ambartsumyan [2]. He showed that if the set of numbers $\lambda_n = (n\pi)^2$ for $n \in \mathbb{N}$ are given as a spectrum of the Sturm-Liouville problem

$$-y'' + q(x)y = \lambda y, \quad x \in (0,1) \tag{1.24}$$

with boundary conditions $y'(0) = 0, \quad y'(1) = 0$ then q is the zero potential, $q = 0$. This result attracts many scientist to make deeper investigation about the existence and uniqueness conditions for the inverse S-L problem. In fact, Ambartsumyan's claim is not true in general, namely the given eigenvalue set is not sufficient to recover a potential uniquely. But it is an exceptional case for symmetric potentials for which one eigenvalue set is enough. The general results were obtained by Borg in 1945 [15]. He showed that if $\{\lambda_n\}$, $n \in \mathbb{N}$ is the eigenvalue set of (1.24) with the boundary conditions $y(0) = 0$, $y(1) = 0$ and if $\{\mu_n\}$, $n \in \mathbb{N}$ is the eigenvalue set of the same equation with different boundary conditions $y'(0) = 0$, $y'(1) = 0$ then the set of eigenpair $\{\lambda_n, \mu_n\}$ uniquely determines the potential $q(x)$ in the equation (1.24). He also showed that if $q(x)$ is symmetric about the line $x = 1/2$, $q(x) = q(1-x)$,

one eigenvalue set is enough for the recovery of q which coincides with the result of [2]. After Borg's paper Levinson published his results in which uniqueness proof was given in a simpler form by using Green's function and complex analysis technique [49]. In 1950 Marchenko [51] showed that if boundary conditions corresponding to $\{\lambda_n\}$ and $\{\mu_n\}$ are given in the form

$$y'(0) - hy(0) = 0, \quad y'(1) + Hy(1) = 0 \tag{1.25}$$

$$y'(0) - hy(0) = 0, \quad y'(1) + H'y(1) = 0, \quad H \neq H' \tag{1.26}$$

then two spectra are sufficient to determine not only potential q but also constants h, H, H' uniquely. After researches about uniqueness via two spectra, Gel'fand and Levitan [28] showed that one spectrum $\{\lambda_n\}_1^\infty$ and a set of norming constants $\{\rho_n\}_1^\infty$ defined by $\rho_n := \frac{\|y_n\|_2^2}{y_n(0)^2}$ for $h \neq 0$, or else $\rho_n := \frac{\|y_n\|_2^2}{y_n'(0)^2}$ for $h = 0$ are enough to recover the potential uniquely. This work showed that it is possible to use other data rather than spectra, but two sequences were required for reconstruction. Hochstadt and Lieberman [37] showed that it is not required any information about second spectrum but instead $q(x)$ is known on the half interval $[1/2, 1]$. This information together with one eigenvalue sequence $\{\lambda_n\}$ is sufficient to determine $q(x)$ uniquely on $[0, 1]$. Another version for this kind of treatment was considered in [38, 39, 62]. They define $\{\kappa_n\}_1^\infty$ known as terminal velocity by means of eigenfunctions, i.e., $\kappa_n := \log\left(\frac{|y_n'(1)|}{|y_n'(0)|}\right)$ if $h = H = \infty$, $\kappa_n := \log\left(\frac{|y_n(1)|}{|y_n'(0)|}\right)$ if $h = \infty$ and $H < \infty$ and showed that $\{\lambda_n\}_1^\infty$ and terminal velocity are able to recover $q(x)$ uniquely. Another version of the inverse problem related with the Sturm-Liouville equation is considered by J. McLaughlin in 1988 [53]. The so-called inverse nodal problem is the problem of reconstructing the potential q and the boundary conditions α, β in (1.3) with $a = 0$, $b = 1$ using only the nodal points $\{x_k^{(n)}\}_1^{n-1}$. Actually these points are $(n-1)$ zeros of the $n-th$ eigenfunction of the Sturm-Liouville equation with associated boundary conditions. She proved that the potential q can be determined up to a constant by means of nodal points of Dirichlet problem. There are several authors studying on the existence, uniqueness and reconstruction process of this kind of problems, see, for example, [18, 25, 31, 47] and references cited therein.

After establishing the existence and uniqueness theory of the inverse Sturm-Liouville problems many authors try to construct an efficient algorithm to get potential from

various set of data. In 1978 Hald [32] proposed an algorithm for solving the inverse Sturm-Liouville problem with symmetric potential and Dirichlet boundary conditions. His algorithm is based on the classical Rayleigh-Ritz method. The main idea under this method is to expand the potential and the eigenfunctions in truncated Fourier series form and reduce the problem to a finite dimensional inverse eigenvalue problem. Namely, he proposed a trial potential

$$q(x) = \alpha_0 + 2\sum_{k=1}^{m} \alpha_k \cos(2kx)$$

and then try to find the coefficients α_k such that the given eigenvalue set $\{\lambda_j\}$ coincides with the eigenvalues of reduced matrix-eigenvalue problem. In this formulation an initial guess for the potential, which was taken basically zero in this work, is needed. Hald showed that the potential converges to a limit potential as the dimension of the space of trial functions is increased. He also observed that continuous and square integrable potentials were reconstructed with less number of eigenvalues whereas discontinuous ones needed more eigenvalues. The success of the algorithm depends on the fact that the matrix and differential eigenvalues have the same asymptotic behaviour. The novelty of this work attracts Paine [59]. He realizes that differential eigenvalues asymptotically behave differently from the eigenvalues of the matrix which is obtained by finite difference method. Paine used the asymptotic correction of finite difference method

$$\epsilon_k = (k^2 - 2h^{-2})(1 - \cos(kh)), \quad k = 1, \ldots, N, \quad h = \pi/(N+1)$$

which has been given in [60]. Actually, by subtracting correction from the differential eigenvalues, one can obtain estimates of the desired finite difference eigenvalues such that they have the same asymptotic behaviour. On the other hand, in the reconstruction procedure Paine used a general form of Sturm-Liouville equation in (1.2) and considered Liouville transformation to pass $q(x)$ from $r(x)$ and $p(x)$ starting with an initial p on a non-uniform mesh. Newton method was taken into account in iterative solution process for a nonlinear system of equations.

In 1990 Marti [52] used finite element discretization and correction technique with Newton Secant method to construct potentials from nonlinear equations

$$\Lambda_k(q) - \overline{\Lambda}_k = 0,\ 1 \le k \le m.$$

In which the eigenvalues $\Lambda_k(q)$ are those of finite element discretization matrix, and $\overline{\Lambda}_k$ are the first m corrected eigenvalues derived from the known eigenvalue set. In addition to these works Pirovino [61] presented convergence result for an inverse algorithm based on a finite difference discretization with an equidistant grid and correction term. Unlike these works, i.e., [32, 52, 59, 61], in which only symmetric potentials, namely $q(x) = q(\pi - x)$ are considered, Fabiano and his co-workers [24] constructed an algorithm for not only symmetric but also general potentials. They used finite number of Dirichlet eigenvalues of the Sturm-Liouville equation on $(0, \pi)$ as spectral data for a symmetric potentials. Finite difference discretization was used to reduce the inverse S-L problem to a matrix inverse eigenvalue problem. Similar nonlinear system of equations in [52] was obtained. But modified Newton's method with a zero potential as a starter was used to solve the nonlinear system. In contrast to the iterative solver in [52] modified Newton's method allows to compute Jacobian matrix one time at the beginning of the first iteration and it uses the same Jacobian through the all iterations. Moreover, it is possible to evaluate Jacobian analytically for zero potential. Their additional data for non-symmetric potentials were terminal velocities which are defined by

$$\kappa_i := \log\left(\frac{|y_i'(\pi)|}{|y_i'(0)|}\right), \quad i = 1, 2, \ldots.$$

The method seeks the zero of the nonlinear map

$$\boldsymbol{H}(q) = [\boldsymbol{U}(q) \quad \boldsymbol{V}(q)]^T$$

for a given spectral set $\{\lambda_i, \kappa_i\}_{i=1}^n$ where

$$\boldsymbol{U}(q) = (\nu_1(q) - \mu_1, \ldots, \nu_n(q) - \mu_n)^T$$

and

$$\boldsymbol{V}(q) = \left(\frac{2\sin(h)}{h}\tau_1(q) - 2\kappa_1, \frac{2\sin(2h)}{h}\tau_2(q) - 4\kappa_2, \ldots, \frac{2\sin(nh)}{h}\tau_n(q) - 2n\kappa_n\right)^T$$

with $\tau_j(q) := \log\left|\frac{[y^j(q)]_{2n}}{[y^j(q)]_1}\right|$. Here $\nu_j(q)$'s are the eigenvalues of the matrix which is obtained from finite difference discretization of the Sturm-Liouville equation with Dirichlet boundary conditions at zero and π, μ_j's are the corrected eigenvalue data, $y^j(q)$ is the j-th eigenvector corresponding to $\nu_j(q)$. The definition of $\boldsymbol{V}(q)$ was attracted by a comparison between the linearization of the matrix data $\tau_j(q)$ and the

Sturm-Liouville data $\kappa_j(q)$. The modified Newton method was used with zero potential as an initial guess for the solution of the nonlinear equation.

In another work [57] an algorithm for symmetric potential on $[0,\pi]$ was presented. Neher tried to construct a potential in the form

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

from the knowledge of the eigenvalue set $(\lambda_i)_{i=1}^n$ and symmetric basis functions $\hat{q}(x)$, $q_j(x)$, $j = 1,\ldots,n$, so that

$$\Lambda_i(q(x;a)) = \lambda_i, \quad i = 1,\ldots,n$$

Thus, inverse problem becomes a finite-dimensional problem of determining $a \in \mathbb{R}^n$ such that the system of n nonlinear equations defined by

$$\boldsymbol{f}(a) = f_i(a) := (\Lambda_i(q(x;a) - \lambda_i)) \quad i = 1,\ldots,n$$

hold. Newton's and interval Newton methods were applied to $\boldsymbol{f}(a) = 0$ to define a reconstruction procedure for recovery of $q(x)$. In this reconstruction procedure a priori information about the potential was required for the choices of $\hat{q}(x)$ and $q_j(x)$. The paper [57] published by the same author in 1998 concerned with the reconstruction of an unknown impedance $p(x)$ in the Sturm-Liouvile problem of the form

$$[p(x)u']' + \lambda p(x)u = 0 \tag{1.27}$$

with Dirichlet boundary conditions $u(0) = u(\pi) = 0$ where the impedance $p(x)$ assumed to be continuously differentiable in $[0,\pi]$, symmetric, i.e., $p(x) = p(\pi - x)$ and positive with $p(0) = 1$. Same techniques as in [56] was used to solve this inverse impedance problem. Shooting method was taken into account to evaluate eigenvalues and eigenfunctions for the direct problem in the iterative solution procedures for both methods in [56] and [57].

In [5] Alan L. Andrew used fourth order Numerov's method to refine the algorithm of [24] which uses second order method. Dirichlet boundary conditions with symmetric potentials on $[0,\pi]$ were considered. In his approaches, for a given finite number of Dirichlet eigenvalues of Sturm-Liouville equation on $[0,\pi]$ he found a vector $\boldsymbol{q} = (q_1, q_2, \ldots q_n)^T$ for which q_i, $i = 1,2,\ldots,n$, is an approximation of symmetric $q(x)$

at the points ih with $h = \frac{\pi}{2n+1}$. Namely q is a solution of the equation $\boldsymbol{f}(q) = 0$ with a starting potential needed in the iterative solution procedure. The components of $\boldsymbol{f}(q)$ are $\Lambda_i(q) + \epsilon_r(i,h) - \lambda_i$ where $\Lambda_i(q)$'s are approximations of λ_i's by means of Numerov's method, and $\epsilon_r(i,h)$ is called an asymptotic correction defined by

$$\epsilon_r(i,h) := \frac{12\sin^2(ih/2)}{h^2[3+(1-r)\sin^2(ih/2)]}.$$

Later Andrew modified this algorithm for non-symmetric potentials with one spectrum plus terminal velocity and symmetric potentials with Neumann boundary conditions [6]. He dealt with Neumann boundary conditions by using either finite difference or Numerov's method. Asymptotic correction was taken as $\epsilon_1(i-1,h)$ for finite difference and $\epsilon_2(i-1,h)$ for Numerov's method with the mesh length $h = \frac{\pi}{2n-1}$. Moreover in [7] he used two spectra associated with different boundary conditions to recover general potentials. However, as is shown in [15] if these boundary conditions differ at only one boundary, then two spectra associated these boundary conditions are sufficient to recover the potential uniquely.

In [7] Andrew used method of symmetric extension which uses the idea under the fact that if $\lambda_i^{(0)}$ and $\lambda_i^{(1)}$ are the eigenvalues of (1.24) with the boundary conditions $y(0) = 0$, $y(\pi) = 0$ and $y(0) = 0$, $y'(\pi) = 0$ respectively then $\lambda_1^{(1)} < \lambda_1^{(0)} < \lambda_2^{(1)} < \lambda_2^{(0)} < \ldots$ are eigenvalues of (1.24) with symmetric potential $q(x) = q(\pi - x)$ and boundary conditions $y(0) = 0$, $y(\pi) = 0$. After this, symmetrically extended potential with one spectra can be reconstructed. At that point it is worth mentioned that the strict interlacing property of eigenvalues is a necessary condition for existence of the solution. Asymptotic corrections for Numerov's method with different boundary conditions were given in [3], [4] and [8] play a key role in his algorithm. The numerical algorithm for partially known potential was given in [42]. Depending on the theory given by Hochstadt and Lieberman [37], Kammanee and Böckmann gave an algorithm to construct a general potential for a given first n exact eigenvalues corresponding to Dirichlet boundary conditions on $[0,\pi]$ and a partially known potential on either $[0,\pi/2]$ or $[\pi/2,\pi]$. They utilized both finite difference and Numerov's method to estimate the desired eigenvalues in each modified Newton iteration step. Again the make up the difference between the asymptotic behaviours of the given and computed eigenvalues, the algebraic (asymptotic) correction was used both methods. In this work, they also used broken eigenvalue set, i.e., the set with a missing eigen-

value. Actually they developed a method depending on the asymptotic behaviour of eigenvalues to recover missing eigenvalue. Furthermore, in [43] Kammanee and Böckmann used boundary value method for the solution of direct problem in the iterative solution procedure. Basically this method converted the equation (1.24) into the system of first order equations $\boldsymbol{u}' = \boldsymbol{A}\boldsymbol{u}$ with

$$\boldsymbol{A} = \begin{bmatrix} 0 & 1 \\ q(x) - \lambda & 0 \end{bmatrix}, \quad \boldsymbol{u} = \begin{bmatrix} u_1(x) \\ u_2(x) \end{bmatrix}$$

where $u_1(x) = y$ and $u_2(x) = y'$ and solved this system. Asymptotic correction was also needed in the reconstruction of potential. More details about boundary value method and the correction terms for this method can be found in [29].

The methods mentioned above up to now use the matrix method. For inverse S-L problems there is another recovery technique which is related with the integral equations. For a given two sets of eigenvalue sequences of (1.24) corresponding to different boundary conditions (1.25) and (1.26) one can construct potential using Gelfand-Levitan- Marchenko operator. This operator is a linear mapping between the solution of equation (1.24) with a known reference potential $p(x)$ and the solution of the same equation with an unknown potential $q(x)$. In other words, let $\mathcal{L}$ and $\tilde{\mathcal{L}}$ be the differential operators for which φ and ψ are solutions of the differential equations

$$\mathcal{L}\varphi = -\varphi'' + q(x)\varphi = \lambda\varphi \qquad \text{and} \qquad \tilde{\mathcal{L}}\psi = -\psi'' + p(x)\psi = \lambda\psi$$

with $q, p \in L^2[0,1]$ satisfying the same conditions at $x = 0$, i.e., $\varphi(0) = \psi(0) = 0$ and $\varphi'(0) = \psi'(0) = 1$. Then the transformation operator T,

$$\varphi(x) = T\psi(x) = \psi(x) + \int_0^1 K(x,t)\psi(t)\mathrm{d}t \tag{1.28}$$

can be obtained [19, 26]. From the well known paper of Gelfand and Levitan [28], there exist a function $K(x,t)$ which is a solution of the Goursat problem

$$K_{tt} - K_{xx} + (q(x) - p(t))K(x,t) = 0, \qquad 0 \le t \le x \le 1$$

$$2\frac{d}{dx}K(x,x) = (q(x) - p(x))$$

$$K(x,0) = 0.$$

Since $K(x,t;p,q)$ does not depend on eigenvalues, Rundell and Sack [69] used this kernel to recover the potential from two sets of eigenvalues. They obtained Cauchy data $K(1,t)$ and $K_x(1,t)$ using the boundary condition at $x=1$, GLM operator (1.28) and given eigenvalue sets. Hence they replaced Goursat problem by a Cauchy problem

$$K_{tt} - K_{xx} = -(q(x) - p(t))K(x,t) \qquad 0 \le |t| \le x \le 1$$

$$K(1,t) = f(t)$$

$$K_x(1,t) = g(t)$$

with the same solution. Note that $K(x,0) = 0$ allows to extend K oddly on the domain $0 \le |t| \le x \le 1$. Thus, $K(x,0) = 0$ holds with odd f and g in $L^2[-1,1]$. They regarded Goursat problem with cauchy data as an overposed boundary value problem for K, and they used this to recover $q(x)$ uniquely. In the reconstruction procedure, Rundell and Sack used zero reference potential, namely $p(x) = 0$ and wrote the D'Alambert solution formula for the inhomogeneous Hyperbolic equation with Cauchy data on $x = 1$ for $K(x,x)$ as

$$K(x,x) = \frac{1}{2}\left[K(1,2x-1) + K(1,1) + \int_1^{2x-1} K_x(1,\xi)d\xi - \int_x^1 \int_{2x-\tau}^{\tau} q(\tau)K(\tau,\xi)d\xi d\tau\right].$$

and they obtained $q(x)$ from the integral equation

$$q(x) = 2\frac{d}{dx}K(x,x) = 2\left[K_t(1,2x-1) + K_x(1,2x-1)\right] - 2\int_x^1 q(\tau)K(\tau,2x-\tau)d\tau$$

by two different iterative procedures which are successive approximation method and Quasi-Newton method. In the first method, they solved the non homogeneous wave equation

$$v_{xx} - v_{tt} = q(x)v \qquad 0 \le |t| \le x \le 1$$

$$v(1,t) = K(1,t), \quad v_x(1,t) = K_x(1,t) \qquad -1 \le t \le 1$$

with an initial q(x) and iterate the solution by

$$q_{n+1} = G(x) - 2\int_x^1 q_n(\tau)v(\tau,2x-\tau,q_n)d\tau$$

in which $G(x) = 2\left[K_t(1,2x-1) + K_x(1,2x-1)\right]$. For the second method, they solved the characteristic initial value problem

$$u_{xx} - u_{tt} = q(x)u \qquad 0 \le |t| \le x \le 1$$

$$u(x,\pm x) = \pm\frac{1}{2}\int_x^0 q(s)ds$$

for a given $q(x)$ and defined the map $\boldsymbol{F}(q) = \{u_t(1;t;q), u_x(1;t;q)\}$. Then the solution q satisfying $\boldsymbol{F}(q) = \{K_t(1;t), K_x(1;t)\}$ was obtained by Quasi-Newton iteration formula

$$q_{n+1} = q_n - (\boldsymbol{DF}(0))^{-1}(\boldsymbol{F}(q_n) - \{K_t(1;t), K_x(1;t)\})$$

where $DF(0)$ denotes the Frechet derivative of F at $q = 0$. Same authors gave a similar algorithm for solving inverse S-L problems in non-potential form (1.27) for $0 < x < 1$ with Dirichlet spectrum, i.e., eigenvalues of S-L problem with $u(0) = u(1) = 0$, and Dirichlet-Neumann spectrum, i.e., eigenvalues of S-L problem with $u(0) = u'(1) = 0$ in [70]. Moreover Sack used Dirichlet spectrum and norming constants

$$\rho_k = \frac{1}{[y_k'(0)]^2}\int_0^1 [y_k(x)]^2 dx$$

in which y_k's are eigenvectors of (1.24) with Dirichlet boundary conditions to recover the potential via GLM operator technique [71]. The usage of the zero reference potential causes small oscillations especially in the discontinuous potentials. In 2007 Rafler and Böckmann [66] modified Rundell-Sack algorithm to minimize this oscillations. They used earlier reconstructions to estimate the jump discontinuity and modified the reference potential with this estimation. Moreover this modified algorithm needs the mean value of the exact potential. They provide the exact mean value of the unknown potential in numerical experiments.

In addition to matrix methods and integral equation related methods functional minimization technique is another type of numerical determination for inverse Sturm-Liouville problems. This technique was conducted in the papers [17] and [68] by Brown and his co-workers and Röhrl respectively. In the first paper, the equation (1.24) was considered with the potential Q and separated boundary conditions

$$\begin{aligned} y(0) + Ay'(0) &= 0 \\ y(1) + By'(1) &= 0. \end{aligned} \tag{1.29}$$

They defined $u_q(x,\lambda)$ and $v_q(x,\lambda)$ as a solutions of (1.24) satisfying the conditions $u_q(0,\lambda) = A$, $u_q'(0,\lambda) = -1$ and $v_q(1,\lambda) = B$, $v_q'(1,\lambda) = -1$ respectively. Then by Sturm-Liouville theory [50] there exist multiplier constants C_n for $n \in \mathbb{N}$ and $0 \le x \le$

1 such that

$$u_Q(x, \lambda_n) = C_n v_Q(x, \lambda_n).$$

These definitions allow them to define the functional $\boldsymbol{G}(q)$ as

$$G(q) = \sum_{n=0}^{N} \omega_n G_n(q)$$

such that $\boldsymbol{G}(Q) = 0$. Where $N > 0$, ω_n's are positive weights and $G_n(q)$ is given by

$$G_n(q) = \int_0^1 \left[(u_q'(x, \lambda_n) - C_n v_q'(x, \lambda_n))^2 + q(u_q(x, \lambda_n) - C_n v_q(x, \lambda_n))^2 \right] \mathrm{d}x.$$

Moreover it was noted that the true potential $Q(x)$ and trial potential $q(x)$ are both positive for all $x \in [0, 1]$. Minimization of $\boldsymbol{G}$ with respect to q by gradient descent method needs Gâteaux derivative of $\boldsymbol{G}$. This derivative was defined by

$$\boldsymbol{G}_n'(q)[h] = \lim_{\epsilon \to 0} \frac{G_n(q + \epsilon h) - G_n(q)}{\epsilon}.$$

After a long calculations based on integration by parts and equation (1.24) they wrote this derivative as

$$\boldsymbol{G}'(q)[h] = \int_0^1 h(x) H(x) \mathrm{d}x$$

where

$$\begin{aligned} H(x) = \Bigg[& 2 \left(u_q \left(v_q - B \frac{u_q + v_q u_q'(1)}{B u_q'(1) + u_q(1)} \right) (u_q'(1) + C) \right. \\ & + v_q \left(u_q - A \frac{u_q v_q'(0) + v_q}{A v_q'(0) + v_q(0)} \right) (C v_q'(0) + 1) C \Bigg) \\ & \left. + (u_q - C v_q)^2 + 2\lambda(-u_q z + C v_q t) \right] \end{aligned} \tag{1.30}$$

is L^2 gradient in which z and t are solutions of

$$\begin{aligned} -z'' + (q - \lambda) z &= u_q - C v_q, \quad z(1) = 0, \, z'(1) = 0, \\ -t'' + (q - \lambda) t &= u_q - C v_q, \quad t(0) = 0, \, t'(0) = 0. \end{aligned}$$

After establishing the derivative it was written

$$\boldsymbol{G}(q + h) = \boldsymbol{G}(q) + \boldsymbol{G}'(q)[h] + O(h^2).$$

Then by taking $h(x) = -H(x)$, there exist α so that the relation $\boldsymbol{G}(q + \alpha h) < \boldsymbol{G}(q)$ holds. This relation reserved them to set up a recovery algorithm by means of a sequence

$$\boldsymbol{G}(q_{m-1} + \alpha_m h_m) < \boldsymbol{G}(q_{m-2} + \alpha_{m-1} h_{m-1}) < \ldots < \boldsymbol{G}(q_{initial} + \alpha_1 h_1).$$

Concisely in the algorithm they set up an initial q and form H_n considering each term in (1.30) depending on n. Then formed

$$h(x) = -\sum_{n=0}^{n_{max}} \omega_n H_n$$

and minimized the final functional

$$\boldsymbol{F}(\alpha) = \boldsymbol{G}(q + \alpha h)$$

to obtain α_{min}. Finally they evaluated the updated potential via

$$q_{j+1} = q_j + \alpha_{min} h$$

to reach the desired accuracy. The spectrum $\{\lambda_n\}_{n=0}^{N}$ of the Sturm-Liouville equation (1.24) with boundary conditions (1.29) together with associated multiplier constants $\{C_n\}_{n=0}^{N}$ for a given N and the boundary parameters A, B in (1.29) were used as initial data. In this formulation, weights ω_n was chosen in a way that the effect of the higher eigenvalues would be less in the recovery procedure than the lower ones. Brown and his research partners used different gradients such as L^∞ and Sobolev type gradients instead of L^2 ones. But L^2 gradient gave more better results than the others. Moreover they reported that the noised data causes some oscillation in the recovered potential.Since they needed the direct solution of (1.24) in the iterative solution method modified Prüfer transform was preferred to obtain the solution with a higher precision. Shortly the equation system

$$\theta' = \sqrt{\lambda} - \frac{q}{\sqrt{\lambda}} \sin^2\theta, \quad \frac{r'}{r} = s^2 \sin\theta\cos\theta\left(1 + \frac{q-\lambda}{s^2}\right)$$

which was obtained by the aforementioned transforms

$$u(x) = \frac{r(x)}{s}\sin\theta(x)$$
$$u'(x) = r(x)s\cos\theta(x)$$
$$s = \lambda^{1/4}$$

was solved numerically instead of (1.24).

In [68] Röhrl gave an algorithm which recovers the potential for the equation (1.24) using two spectrum associated with different boundary conditions via functional minimization. Röhrl defined a least square functional

$$\boldsymbol{G}(q) = \sum_{i,n} \omega_{i,n}(\lambda_{q,i,n} - \lambda_{Q,i,n})^2, \quad n \in \mathbb{N}_0, \quad i = 1, 2$$

for trial potential q and positive weights $\omega_{i,n}$. Where $\lambda_{Q,i,n}$ are given spectrums and $\lambda_{q,i,n}$ are eigenvalues for trial potential. It was known from [21], [50] and [77] that interlacing property of eigenvalues and correct asymptotics are sufficient for the existence of potential q with $\boldsymbol{G}(q) = 0$. Röhrl also showed that all critical points of this functional occur at global minima. This fact allows him to minimize the least square functional $\boldsymbol{G}(q)$ by a conjugate gradient descent algorithm. In brief for a chosen initial potential q_0, the gradient

$$\nabla \boldsymbol{G}(q) = 2 \sum_{i,n} (n+1)\omega_{i,n}(\lambda_{q,i,n} - \lambda_{Q,i,n}) \frac{1}{n+1} g_{q,i,n}^2$$

was computed to minimize the functional $\boldsymbol{G}(q_i - \alpha \nabla \boldsymbol{G}(q_i))$ with respect to α. Where $\boldsymbol{g}_{q,i,n}$ denotes the normalized eigenfunction corresponding to $\lambda_{q,i,n}$. When $\boldsymbol{G}(q_i)$ is sufficiently small, q_{i+1} is to be taken as an approximating potential. Röhrl was chosen $\omega_{i,n} = 1$, $q_0 = 0$ and was taken 30 eigenvalue pairs with Dirichlet and mixed boundary conditions in his numerical experiments.

CHAPTER 2

REGULARIZATION OF ILL-POSED PROBLEMS

Inverse problems such as Radon inversion (X-ray tomography), signal and image processing, inverse heat conduction, parameter identification, inverse scattering frequently lead to mathematical models which do not satisfy the Hadamard postulates of well-posedness, i.e., they might not have a solution, or solution may not be unique or solutions might not depend continuously on the initial data. This violation is considered as ill-posedness in the Hadamard sense. The numerical solution of ill-posed problems is unstable under data perturbations. Thus, the classical methods often fail to get a solution of such a problems. On the other hand, even if a problem is well-posed it may still be ill-conditioned which means the small perturbations in the initial data can cause the large errors in the solution. Unfortunately no mathematical techniques exist to transform the mentioned unstable problems to stable one. But it is possible to built an agreement between the accuracy and stability via regularization techniques. Thus, the art of the regularization methods is to recover a partial information about the solution as stable as possible.

2.1 Ill-Posed Linear Operator Equations

In this chapter we firstly consider a linear operator equation of the form

$$Tx = y \tag{2.1}$$

where X and Y are Hilbert spaces and T is a bounded linear operator from X to Y. We consider that y is attainable if $y \in \mathcal{R}(T)$. Here $\mathcal{R}(T)$ stands for the range of T. Then every $y \in Y$ being attainable is equivalent to the existence of the solution, and

uniqueness of the solution is valid if and only if $\mathcal{N}(T) = \{0\}$ where $\mathcal{N}(T)$ is the null space of T. Thus, if existence and uniqueness conditions hold so that the inverse operator T^{-1} exists. Moreover, the continuously dependence of the solution to the data equivalent to continuity (or boundedness) of T^{-1}. As a consequence if the equation (2.1) is well-posed then T has a well-defined, continuous inverse operator T^{-1}. But these conditions, i.e., attainability of y and $\mathcal{N}(T) = \{0\}$, would be too restrictive. If $\mathcal{N}(T) \neq \{0\}$ which means the solutions of (2.1) are not unique it should be possible to be interested in a specific solution satisfying additional requirements. Or it is possible to seek a generalized solution even if y is not attainable. This generalized solution will be provided by means of the concept of a generalized inverse of T. Then the last condition of the Hadamard's well-posedness will be relevant to the continuity of the generalized inverse of T.

2.1.1 The Moore-Penrose Generalized Inverse

Definition 2.1 *Let $T : X \longrightarrow Y$ be a bounded linear operator.*

(i) $x \in X$ is called least-squares solution of $Tx = y$ if

$$\|Tx - y\|_Y = inf\{\|Tz - y\|_Y \mid z \in X\} \tag{2.2}$$

(ii) $x \in X$ is called best-approximate solution of $Tx = y$ if x is a least-squares solution of $Tx = y$ and

$$\|x\|_X = inf\{\|z\|_X \mid z \text{ is least squares solution of } Tx = y\} \tag{2.3}$$

holds.

Basically the best approximate solution is defined as the least-squares solution of minimal norm. The definition of the Moore-Penrose inverse can be done by restricting the domain and range of T in such a way that the resulting restricted operator is invertible and its inverse will then be extended to its maximal domain.

Definition 2.2 *The Moore-Penrose generalized inverse $T^\dagger$ of a linear operator T is defined as the unique linear extension of $\tilde{T}^{-1}$ to*

$$\mathcal{D}(T^\dagger) := \mathcal{R}(T) + \mathcal{R}(T)^\perp \quad \text{with} \quad \mathcal{N}(T^\dagger) = \mathcal{R}(T)^\perp$$

where

$$\tilde{T} := T|_{\mathcal{N}(T)^\perp} : \mathcal{N}(T)^\perp \longrightarrow \mathcal{R}(T).$$

The Moore Penrose generalized inverse $T^\dagger$ and best approximate solution are closely related. Actually $T^\dagger$ is a solution operator mapping y onto the best approximate solution of $Tx = y$.

Theorem 2.3 *([23], Theorem 2.5) Let $y \in \mathcal{D}(T^\dagger)$. Then $Tx = y$ has a unique best approximate solution, which is given by*

$$x^\dagger := T^\dagger y$$

Theorem 2.4 *([23], Theorem 2.6) Let $y \in \mathcal{D}(T^\dagger)$. Then $x \in X$ is a least-squares solution of $Tx = y$ if and only if the normal equation*

$$T^*Tx = T^*y$$

holds.

Consequently by virtue of definition (2.1), theorem (2.3) and theorem (2.4), $T^\dagger y$ is the solution of $T^*Tx = T^*y$ of minimal norm, i.e.,

$$T^\dagger = (T^*T)^\dagger T^*$$

2.1.2 Compact Linear Operators

An operator $T : X \longrightarrow Y$ between normed spaces is called a compact operator if it transforms bounded sets in the space X to relatively compact sets in the space Y.

Example 2.5 *Any linear operator $T : X \longrightarrow Y$ for which $\mathcal{R}(T)$ is finite dimensional is compact. In particular, matrix operators are compact.*

Theorem 2.6 *([78], Theorem 2.14) Let $T : X \longrightarrow Y$ be a compact linear operator, and let X and Y be infinite dimensional. If $\mathcal{R}(T)$ is infinite dimensional, then the operator equation $Tx = y$ is ill-posed in the sense that the first and third conditions*

of the Hadamard definition of well-posedness are violated. In this case $\mathcal{R}(T)$ is not closed. If $\mathcal{R}(T)$ has finite dimension, then the second condition of the Hadamard definition of well-posedness is violated.

Example 2.7 *Let us consider the linear system $Ax = y$, $A : \mathbb{R}^n \longrightarrow \mathbb{R}^m$. This system has a unique solution $x^\dagger := A^\dagger y$ if A^TA is non-singular. Here we define $A^\dagger = (A^TA)^{-1}A^T$. And since the operator A is defined on finite dimensional spaces it is always continuous. Thus, the problem $(A, \mathbb{R}^n, \mathbb{R}^m)$ is well-posed.*

Now let X and Y be Hilbert spaces. Define the operator $A : X \longrightarrow Y$ satisfying

$$Af = g \tag{2.4}$$

If we multiply (2.4) with the adjoint operator of A, A^*, we get

$$A^*Af = A^*g \tag{2.5}$$

If we define $f^\dagger = A^\dagger g$ then $f^\dagger$ is a unique solution of (2.5). But in general $A^\dagger$ is discontinuous and unbounded. This means that (A, X, Y) will be ill-posed. Moreover let us consider more precise example to emphasize the usage of the word "in general".

We consider the problem

$$Af(x) := \int_0^x f(t)dt = g(x), \quad x \in [0, 1]. \tag{2.6}$$

The equation (2.6) has unique solution if and only if $g \in C^1_*(0, 1) = \left\{ f \in C^1(0, 1) \mid f(0) = 0 \right\}$ where $C^1(0, 1)$ denotes the set of all continuously differentiable functions on the interval $(0, 1)$. By the Fundamental Theorem of Calculus $f = g'$. The integral operator $A : C(0, 1) \longrightarrow C^1_*(0, 1)$ in equation (2.6) is bijective, and its inverse A^{-1} is continuous. Here $C(0, 1)$ denotes the set of all continuous functions on $(0, 1)$. Then we write

$$\begin{aligned} \|Af\|_{C^1(0,1)} &= \sup_{x\in[0,1]} |Af(x)| + \sup_{x\in[0,1]} |(Af)'(x)| \\ &= \sup_{x\in[0,1]} |Af(x)| + \sup_{x\in[0,1]} |f(x)| \\ &\geq \sup_{x\in[0,1]} |f(x)| \\ &= \|f\|_{C(0,1)} \end{aligned}$$

and obtain

$$\frac{\|Af\|_{C^1(0,1)}}{\|f\|_{C(0,1)}} = \|A\| \geq 1 \Rightarrow \|A^{-1}\| \leq 1$$

which proves the boundedness of A^{-1}. Thus, $(A, C(0,1), C^1_*(0,1))$ is well posed.

Next, let us consider the problem $(A, \mathcal{L}^\infty(0,1), \mathcal{L}^\infty(0,1))$ where $\mathcal{L}^\infty(0,1)$ is the set of all essentially bounded functions on $(0,1)$ with the norm $\|f\| = \operatorname{ess\,sup}_{x\in[0,1]} |f(x)|$ for which there exist a positive constant C, satisfying $|f(x)| < C$ for almost all $x \in (0,1)$, is called essential supremum (ess sup) of $f \in \mathcal{L}^\infty(0,1)$. And let A be the same operator as in (2.6). Let us define the equation

$$Af = g^\varepsilon \tag{2.7}$$

in which g^ε is noisy function having $g^\varepsilon(0) = \varepsilon(0) \neq 0$, i.e., $g^\varepsilon \notin C^1_*(0,1)$. Now if we choice the special noisy function as

$$g^\varepsilon(x) = g(x) + \varepsilon \sin nx,\ \varepsilon > 0$$

we will have $\|g^\varepsilon - g\|_{\mathcal{L}^\infty} = \varepsilon$ and $\|f^\varepsilon - f\|_{\mathcal{L}^\infty} = \|(g^\varepsilon)' - g'\|_{\mathcal{L}^\infty} = \varepsilon n$ in which f^ε is called noisy solution. Finally the special noise ε defined by $\varepsilon = \varepsilon_n = \frac{1}{\sqrt{n}}$ gives

$$\|g^{\varepsilon_n} - g\|_{\mathcal{L}^\infty} = \varepsilon_n = \frac{1}{\sqrt{n}} \to 0$$

and

$$\|f^{\varepsilon_n} - f\|_{\mathcal{L}^\infty} = \varepsilon_n n = n\frac{1}{\sqrt{n}} = \sqrt{n} \to \infty$$

when $n \to \infty$ and $\varepsilon \to 0$. This means $A : \mathcal{L}^\infty(0,1) \longrightarrow \mathcal{L}^\infty(0,1)$ has no continuous and bounded inverse. Thus, $(A, \mathcal{L}^\infty(0,1), \mathcal{L}^\infty(0,1))$ is ill-posed problem.

2.1.3 Singular Value Expansion

Let A be self-adjoint compact operator on a Hilbert space X. Then there exist a sequence $\{\lambda_j\}_{j\in\mathbb{N}}$ in $\mathbb{R}$ with $|\lambda_1| \geq |\lambda_2| \geq \ldots \geq 0$ and an orthonormal set of functions $\{v_j\}_{j\in\mathbb{N}}$ in X such that

$$Ax = \sum_{j=1}^{\infty} \lambda_j \langle x, v_j\rangle_X v_j.$$

The elements of the sequences $\{\lambda_j\}_{j\in\mathbb{N}}$ and $\{v_j\}_{j\in\mathbb{N}}$ are called eigenvalues and corresponding eigenvectors of A respectively. The system $(\lambda_j, v_j)_{j\in\mathbb{N}}$ is called eigensystem of A.

In general the operator A might not be self-adjoint. But since A^*A is self- adjoint on X for a compact operator A between Hilbert spaces X and Y we may write

$$A^*Ax = \sum_{j=1}^{\infty} \lambda_j \langle x, v_j \rangle_X v_j$$

with $\lambda_j \in \sigma(A^*A) - \{0\}$(or $\lambda_j \in \sigma(AA^*) - \{0\}$) and corresponding eigenvector v_j in X. Then we have

$$\lambda_j \|v_j\|_X^2 = \langle \lambda_j v_j, v_j \rangle_X = \langle A^*Av_j, v_j \rangle_X = \langle Av_j, Av_j \rangle_Y = \|Av_j\|_Y^2 > 0$$

which implies $\lambda_j > 0$, $j \in \mathbb{N}$. Now Let us define

$$\sigma_j := \sqrt{\lambda_j} \quad \text{and} \quad u_j := \frac{1}{\sigma_j} Av_j, \ j \in \mathbb{N}.$$

Then $Av_j = \sigma_j u_j$ and from this relation we get

$$A^*u_j = A^* \frac{1}{\sigma_j} Av_j = \frac{1}{\sigma_j} \sigma_j^2 v_j = \sigma_j v_j \Rightarrow A^*u_j = \sigma_j v_j, \ j \in \mathbb{N}.$$

Since

$$\begin{aligned} \langle u_j, u_k \rangle_Y = \frac{1}{\sigma_j \sigma_k} \langle Av_j, Av_k \rangle_Y &= \frac{1}{\sigma_j \sigma_k} \langle A^*Av_j, v_k \rangle_X \\ &= \frac{1}{\sigma_j \sigma_k} \langle \lambda_j v_j, v_k \rangle_X = \frac{\sigma_j}{\sigma_k} \langle v_j, v_k \rangle_X = \delta_{jk} \end{aligned}$$

and

$$\|u_j\|_Y^2 = \frac{1}{\sigma_j^2} \langle Av_j, Av_j \rangle_Y = \frac{1}{\sigma_j^2} \langle A^*Av_j, v_j \rangle_X = \frac{1}{\sigma_j^2} \langle \lambda_j v_j, v_j \rangle_X = \|v_j\|_x^2,$$

where $\{v_j\}_{j \in \mathbb{N}}$ is an orthonormal set.

Definition 2.8 *Let $A : X \longrightarrow Y$ be a compact operator between Hilbert spaces X and Y. The triple $(\sigma_j, v_j, u_j)_{j \in \mathbb{N}} \subset (0, \infty) \times X \times Y$ is called singular system of the operator A. Here σ_j, v_j, u_j are called singular values, right eigenvectors and left eigenvectors of A^*A respectively.*

And by using singular system we obtain the so-called singular value expansion(SVE) of A;

$$Ax = \sum_{j=1}^{\infty} \sigma_j \langle x, v_j \rangle_X u_j \, , x \in X.$$

For the adjoint operator, the singular value expansion takes the form;

$$A^*y = \sum_{j=1}^{\infty} \sigma_j \langle y, u_j \rangle_Y v_j \, , y \in Y.$$

In this subsection we conclude finally that for $g \in \mathcal{D}(A^\dagger)$, the least square solution of (2.4) with minimal norm is given by the formula

$$f^\dagger = A^\dagger g = \sum_{j=1}^{\infty} \sigma_j^{-1} \langle g, u_j \rangle_Y v_j. \tag{2.8}$$

We call the equation (2.8) the singular value expansion of the Moore-Penrose generalized inverse $A^\dagger$ where $(\sigma_j, v_j, u_j)_{j\in\mathbb{N}}$ is the singular system of A. Moreover it is important to check the convergence condition of the singular value expansion. This convergence criteria for this expansion, namely,

$$\sum_{j=1}^{\infty} \frac{1}{\sigma_j^2} |\langle g, u_j \rangle_Y|^2 < \infty$$

is called the Picard criteria. Indeed the best approximate solution exists only if the coefficients $(\langle g, u_j \rangle_Y)$ with respect to the singular functions u_j decay fast enough relative to the singular values σ_j.

At this point it is worth mentioned that if $\mathcal{R}(A)$ is infinite dimensional, then the singular values $\{\sigma_j\}_{j\in\mathbb{N}}$ have the following additional property.

$$\lim_{n\to\infty} \sigma_n = 0.$$

The representation of $A^\dagger g$ in (2.8) shows that $A^\dagger$ is unbounded if $\mathcal{R}(A)$ is infinite dimensional.

On the other hand, equation (2.8) shows how errors in data g affect the solution $A^\dagger g$. Namely, error components (with respect to the basis u_n) corresponding to the large singular values are harmless. However, error components corresponding to the small singular values are dangerous because of the factor $\frac{1}{\sigma_n}$. If $\mathcal{R}(A)$ is finite dimensional then there are only finitely many singular values so that the amplification factors $\frac{1}{\sigma_n}$ are at least bounded, although they might still be unacceptably large. If $\mathcal{R}(A)$ is infinite dimensional, i.e., $\lim_{n\to\infty} \sigma_n = 0$ holds then $\frac{1}{\sigma_n}$ increases without bound.

2.2 Regularization Theory

In this section our aim is to approximate the best-approximate solution $x^\dagger = T^\dagger y$ of (2.1) for a given right hand side y. Most problems in the inverse problem theory

the exact data y are not available accurately, but that an approximate data y^ε with $\|y^\varepsilon - y\| \leq \varepsilon$ are known. In the context of the literature y^ε and ε are called noisy data and noise level respectively.

If the equation (2.1) is ill-posed, $T^\dagger y^\varepsilon$ does not serve a good approximation of $T^\dagger y$ because of the unboundedness of $T^\dagger$. We require some approximate solution, say x_γ^ε, of $x^\dagger$, depends continuously on the given noisy data y^ε so that it can be computed in a stable way. Here γ is called regularization parameter which will be chosen suitably such that x_γ^ε tends to $x^\dagger$ as the noise level ε decreases to zero. The solution process for x_γ^ε is in general related with the operator T. This says that we do not only deal with to regularize the specific equation but also with the regularizing the solution operator $T^\dagger$. Intuitively a regularization of the operator $T^\dagger$ should be the replacement the unbounded operator by a parameter dependent family R_γ of continuous operators. Then we take $x_\gamma^\varepsilon := R_\gamma y^\varepsilon$ as an approximation of $x^\dagger$.

Definition 2.9 *Let $T : X \longrightarrow Y$ be a bounded linear operator between the Hilbert spaces X and Y and let $\{R_t\}_{t>0}$ be a family of continuous (not necessarily linear) operators mapping Y into X with $R_t 0 = 0$. If for all $y \in \mathcal{D}(T^\dagger)$ there exist one mapping $\gamma : \mathbb{R}^+ \times Y \longrightarrow (0, \gamma_0)$, $\gamma_0 \in (0, \infty)$ such that*

$$\limsup_{\varepsilon \to 0} \left\{ \|T^\dagger y - R_{\gamma(\varepsilon, y^\varepsilon)} y^\varepsilon\|_X \ : \ y^\varepsilon \in Y \, , \, \|y - y^\varepsilon\| \leq \varepsilon \right\} = 0 \tag{2.9}$$

and

$$\limsup_{\varepsilon \to 0} \{\gamma(\varepsilon, y^\varepsilon) \ : \ y^\varepsilon \in Y \, , \, \|y - y^\varepsilon\| \leq \varepsilon\} = 0 \tag{2.10}$$

hold. Then we call the family $\{R_\gamma\}$ a regularization or a regularization operator for $T^\dagger$. The parameter $\gamma = \gamma(\varepsilon, y^\varepsilon)$ is called regularization parameter and the pair (R_γ, γ) is called a (convergent) regularization method for (2.1) if (2.9) and (2.10) hold.

In particular, R_γ are linear then we call the corresponding method is a linear regularization method and the family $\{R_\gamma\}$ be a linear regularization operator.

Now, let y^ε be a perturbed version of the exact data y satisfying $\|y - y^\varepsilon\| \leq \varepsilon$ with noise level ε and let $x_t^\varepsilon = R_t y^\varepsilon$ be an approximation of the best approximate solution $x^\dagger = T^\dagger y$ of (2.1). Where $\{R_t\}_{t>0}$ is a family of continuous linear operators. The total

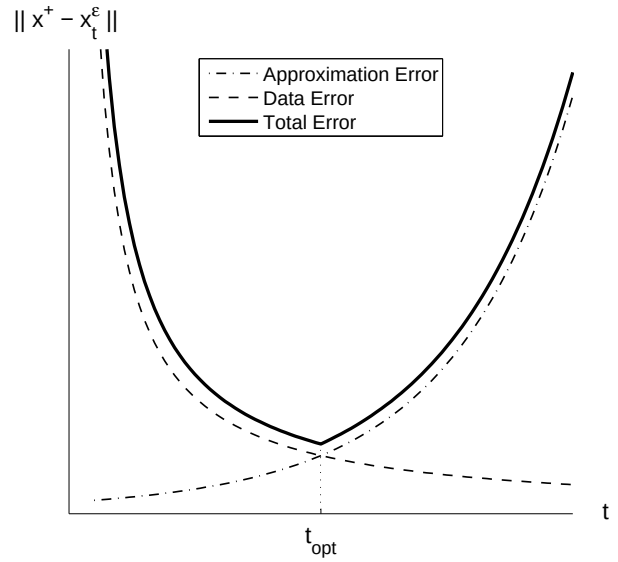

Figure 2.1: The behaviour of the total error in the regularization procedure

error can be written as

$$\begin{aligned} \|x^\dagger - x_t^\varepsilon\| = \|T^\dagger y - R_t y^\varepsilon\| &= \|T^\dagger y - R_t y + R_t y - R_t y^\varepsilon\| \\ &\leq \|T^\dagger y - R_t y\| + \|R_t y - R_t y^\varepsilon\| \\ &= \|(T^\dagger - R_t)y\| + \|R_t(y - y^\varepsilon)\|. \end{aligned}$$

The first part is called an approximation error and the other part is called data error. When $t \to 0$ the approximation error tends to 0 while the data error tends to ∞. Figure (2.1) shows the behaviour of the total error. It can be seen from the figure that the total error can never be zero. We need to determine an optimal regularization parameter $t_{opt.}$ which minimizes the total error. Determination of such a parameter is the task of the parameter choice rule. From this point of view we want to select a partial set $\{\gamma = \gamma(\varepsilon, y^\varepsilon)\}$ from the parameter set $\{t > 0\}$ for which $\|T^\dagger y - R_{\gamma(\varepsilon,y^\varepsilon)} y^\varepsilon\| \to 0$ if the noise level approaches to zero.

Definition 2.10 *(Filter Function) Let $\{g_t\}_{t>0}$ be a family of at least piecewise continuous functions. The function $g_t : [0, \|T\|^2] \longrightarrow \mathbb{R}$ satisfying $\lim_{t\to 0} g_t(\lambda) = \frac{1}{\lambda}$ and $\lambda|g_t(\lambda)| < C$ for all $\lambda \in (0, \|T\|^2]$ and $C > 0$ is called Filter function (or filter factor).*

Now we define the regularization operator via filter function and singular value ex-

pansion of T as follows.

$$R_t y := g_t(T^*T)T^*y = \sum_{k=1}^{\infty} g_t(\sigma_k^2)\sigma_k \langle y, u_k\rangle_Y v_k. \tag{2.11}$$

Different choices of the filter function in this formulation lead to the different regularization methods.

Theorem 2.11 *Let for all $\gamma > 0$, $g_\gamma : [0, \|T\|^2] \longrightarrow \mathbb{R}$ be a filter function. Then*

$$\lim_{\gamma\to 0} g_\gamma(T^*T)T^*y = \begin{cases} T^\dagger y & \text{if} \quad y \in D(T^\dagger) \\ \infty & \text{if} \quad y \notin D(T^\dagger) \end{cases}$$

Example 2.12 *Let*

$$g_\gamma(\lambda) = \begin{cases} \frac{1}{\lambda} & , \quad \lambda \geq \gamma \\ 0 & , \quad \lambda < \gamma \end{cases}$$

with $\gamma > 0$ and $\lambda \in [0, \|T\|^2]$. Then we obtain

$$\begin{aligned} R_\gamma y &= g_\gamma(T^*T)T^*y \\ &= \sum_{k=1}^{\infty} g_t(\sigma_k^2)\sigma_k \langle y, u_k\rangle_Y v_k \\ &= \sum_{\sigma_k^2 \geq \gamma} (\sigma_k)^{-1} \langle y, u_k\rangle_Y v_k. \end{aligned}$$

Since $\lambda |g_t(\lambda)| = 1$ and $\lim_{t\to 0} g_t(\lambda) = \frac{1}{\lambda}$ by theorem (2.11

$$R_\gamma y = \sum_{\sigma_k^2 \geq \gamma} (\sigma_k)^{-1} \langle y, u_k\rangle_Y v_k \to T^\dagger y. \tag{2.12}$$

It follows from the sum in (2.12) that we filter many singular values and use the first few ones and the corresponding singular functions. This is agree with the characteristics of the singular value decomposition. The regularization operator in (2.12) leads to the so called truncated singular value decomposition regularization method.

Definition 2.13 *For a given noisy data y^ε satisfying $\|y^\varepsilon - y\| \leq \varepsilon$, if the regularization parameter γ should be chosen only depending on ε then we call this choosing strategy as an a-priori rule. Otherwise, it is called an a-posteriori parameter choice rule. Thus, an a-priori parameter choice rule depends only on the noise level while an a-posteriori rule depends on actual data and estimation of noise level.*

Moreover the noise level information may not be available for some inverse problems. Therefore it is necessary to consider alternative parameter choice rules that does not require the knowledge of the noise level. Such heuristic parameter choice rules are called error free parameter choice rules.

2.2.1 Tikhonov-Philips Regularization

For a compact operator T between Hilbert spaces X and Y, T^*T is a self-adjoint compact operator with non-negative eigenvalues. If γ is any positive number then the operator $(T^*T + \gamma I)$ has strictly positive eigenvalues. Since the operator $(T^*T + \gamma I)$ has a bounded inverse, the problem of solving the equation

$$(T^*T + \gamma I)x_\gamma = T^*y \tag{2.13}$$

is well-posed. The equation (2.13) is called a regularized form of the normal equation. The unique solution

$$x_\gamma = (T^*T + \gamma I)^{-1}T^*y \tag{2.14}$$

of equation (2.13) is called the Tikhonov (or Tikhonov-Philips) approximation to $T^\dagger y$. The method which gives the solution (2.14) is called Tikhonov-Philips regularization method. Now let us show that the Tikhonov approximation x_γ converge to $T^\dagger y$ as $\gamma \to 0$. First of all for a given singular system $(\sigma_j, v_j, u_j)_{j\in\mathbb{N}}$ of T, $\{v_j\}$ is a complete orthonormal set of eigenvectors for $\mathcal{R}(T^*T) = \mathcal{N}(T)^\perp$ and $\{u_j\}$ is a complete orthonormal set of eigenvectors for $\mathcal{R}(TT^*) = \mathcal{N}(T^*)^\perp$. From equation (2.13) we write

$$\gamma x_\gamma = T^*y - T^*Tx_\gamma$$

and hence we get $x_\gamma \in \mathcal{R}(T^*) \subset \overline{\mathcal{R}(T^*)} \subset \mathcal{N}(T)^\perp$. Therefore we may expand $x_\gamma \in \mathcal{N}(T)^\perp$ in terms of the singular vectors $\{v_j\}$ which constitutes an orthonormal basis for $\mathcal{N}(T)^\perp$ as follows:

$$x_\gamma = \sum_{j=1}^{\infty} \langle x_\gamma, v_j\rangle_X v_j. \tag{2.15}$$

Similarly, we may expand $T^*y \in \mathcal{R}(T^*) \subset \overline{\mathcal{R}(T^*)} \subset \mathcal{N}(T)^\perp$ in terms of the singular vectors $\{v_j\}$ as

$$T^*y = \sum_{j=1}^{\infty} \langle T^*y, v_j\rangle_X v_j = \sum_{j=1}^{\infty} \langle y, Tv_j\rangle_Y v_j = \sum_{j=1}^{\infty} \langle y, \sigma_j u_j\rangle_Y v_j = \sum_{j=1}^{\infty} \sigma_j \langle y, u_j\rangle_Y v_j \tag{2.16}$$

by using the definition of u_j, i.e., $u_j := \frac{1}{\sigma_j} T v_j$. Now if we substitute (2.15) and (2.16) in (2.13) we obtain

$$\begin{aligned}
\sum_{j=1}^{\infty} \sigma_j \langle y, u_j \rangle_Y v_j &= \sum_{j=1}^{\infty} \langle T^* T x_\gamma, v_j \rangle_X v_j + \sum_{j=1}^{\infty} \gamma \langle x_\gamma, v_j \rangle_X v_j \\
&= \sum_{j=1}^{\infty} \langle x_\gamma, T^* T v_j \rangle_X v_j + \sum_{j=1}^{\infty} \gamma \langle x_\gamma, v_j \rangle_X v_j \\
&= \sum_{j=1}^{\infty} \langle x_\gamma, \sigma_j^2 v_j \rangle_X v_j + \sum_{j=1}^{\infty} \gamma \langle x_\gamma, v_j \rangle_X v_j \\
&= \sum_{j=1}^{\infty} \sigma_j^2 \langle x_\gamma, v_j \rangle_X v_j + \sum_{j=1}^{\infty} \gamma \langle x_\gamma, v_j \rangle_X v_j \\
&= \sum_{j=1}^{\infty} (\sigma_j^2 + \gamma) \langle x_\gamma, v_j \rangle_X v_j.
\end{aligned}$$

Here we use the identity $T^* T v_j = \lambda_j v_j = \sigma_j^2 v_j$. Hence we obtain

$$\langle x_\gamma, v_j \rangle_X = \frac{\sigma_j}{\sigma_j^2 + \gamma} \langle y, u_j \rangle_Y. \tag{2.17}$$

Thus, using (2.17) in (2.15) we get

$$x_\gamma = \sum_{j=1}^{\infty} \frac{\sigma_j}{\sigma_j^2 + \gamma} \langle y, u_j \rangle_Y v_j. \tag{2.18}$$

Since the least-squares solution is given by

$$T^\dagger y = \sum_{j=1}^{\infty} \frac{1}{\sigma_j} \langle y, u_j \rangle_Y v_j$$

it is possible to write

$$\begin{aligned}
\| x_\gamma - T^\dagger y \|^2 &= \left\| \sum_{j=1}^{\infty} \left(\frac{\sigma_j}{\sigma_j^2 + \gamma} - \frac{1}{\sigma_j} \right) \langle y, u_j \rangle_Y v_j \right\|^2 \\
&= \sum_{j=1}^{\infty} \left(\frac{1}{\sigma_j} - \frac{\sigma_j}{\sigma_j^2 + \gamma} \right)^2 \left| \langle y, u_j \rangle_Y \right|^2 \\
&\leq \sum_{j=1}^{\infty} \frac{1}{\sigma_j^2} \left| \langle y, u_j \rangle_Y \right|^2 \\
&= \left\| T^\dagger y \right\|^2 < \infty
\end{aligned}$$

and

$$\lim_{\gamma \to 0} \| x_\gamma - T^\dagger y \|^2 = \lim_{\gamma \to 0} \sum_{j=1}^{\infty} \left(\frac{1}{\sigma_j} - \frac{\sigma_j}{\sigma_j^2 + \gamma} \right)^2 \left| \langle y, u_j \rangle_Y \right|^2 = 0.$$

Therefore $x_\gamma \to T^\dagger y$ as $\gamma \to 0$.

On the other hand, if we compare (2.11) and (2.18) we can easily see that the filter function $g_\gamma(\lambda) = \frac{1}{\lambda+\gamma}$ produces the Tikhonov-Philips regularization method.

Definition 2.14 *Let $T : X \longrightarrow Y$ be a bounded linear operator between the Hilbert spaces X and Y. For a given positive γ the functional defined by*

$$\mathcal{F}_\gamma(x) = \|Tx - y\|_Y^2 + \gamma\|x\|_X^2$$

is called Tikhonov functional.

At this point it is possible to give the uniqueness of the solution of (2.1) via Tikhonov functional.

Theorem 2.15 *Let $T : X \longrightarrow Y$ be a bounded linear operator between the Hilbert spaces X and Y and x_γ be given as in (2.14) with $\gamma > 0$. Then the Tikhonov functional $\mathcal{F}_\gamma(x) = \|Tx - y\|_Y^2 + \gamma\|x\|^2$ has a unique minimizer x_γ.*

Proof. See [44]. □

Remark 2.16 *It is possible to choose Tikhonov functional $\mathcal{F}$ as*

$$\mathcal{F}_\gamma(x) = \|Tx - y\|_Y^2 + \gamma\|Lx\|_X^2$$

where L is called regularization operator on Hilbert space X. The choice of this kind of functional leads to the minimizer

$$x_\gamma = (T^*T + \gamma L^*L)^{-1}T^*y \tag{2.19}$$

as a regularized solution of the problem (2.1). The method which produces the solution (2.19) is called generalized Tikhonov-Philips regularization. Moreover we can transform the problem

$$min\left\{\|Tx - y\|_Y^2 + \gamma^2\|Lx\|_X^2\right\}$$

to a standard form in which L is identity operator. Actually, if L is invertible then with $\overline{T} = TL^{-1}$, $\overline{x} = Lx$ we can solve the equivalent system

$$min\left\{\|\overline{T}\overline{x} - y\|_Y^2 + \gamma^2\|\overline{x}\|_X^2\right\}.$$

The effect of the regularization operator will be presented in the numerical results. But, basically it penalizes the non smooth solutions. Thus, L can be chosen to be the discretization of the derivative operators [33].

The selection of the regularization parameter is very crucial for the achievement of the method. If too much regularization is imposed on the solution then the residual $\|Tx - y\|_Y$ will be too large. On the other hand, if regularization is too little then the solution is dominated by the data errors.

2.2.2 Discrepancy Principle

The discrepancy principle is a-posteriori stopping rule which determines the regularization parameter considering the balance between the data and approximation errors.

Definition 2.17 *(Discrepancy Principle) Let $g_\gamma : [0, \|T\|^2] \longrightarrow \mathbb{R}$ be a filter function and satisfies Theorem 2.11. Moreover let r_γ be defined by $r_\gamma(\lambda) := 1 - \lambda g_\gamma(\lambda)$ and let*

$$\tau > sup\left\{|r_\gamma(\lambda)| \mid \gamma > 0,\ \lambda \in [0, \|T\|^2]\right\}. \tag{2.20}$$

Now the regularization parameter defined by discrepancy principle is

$$\gamma(\varepsilon, y^\varepsilon) := sup\left\{\gamma > 0 \mid \|Tx_\gamma^\varepsilon - y^\varepsilon\| \leq \tau\varepsilon\right\} \tag{2.21}$$

We assume that for each $\lambda > 0$, $\gamma \to g_\gamma(\lambda)$ is continuous from left, so that also the functional $\gamma \to \|Tx_\gamma^\varepsilon - y^\varepsilon\|$ is continuous from the left. Consequently the supremum in (2.21) is attained, so that

$$\|Tx^\varepsilon_{\gamma(\varepsilon,y^\varepsilon)} - y^\varepsilon\| \leq \tau\varepsilon.$$

If $\|Tx_\gamma^\varepsilon - y^\varepsilon\| \leq \tau\varepsilon$ for all $\gamma > 0$, then $\gamma(\varepsilon, y^\varepsilon) = \infty$. Thus, the regularization parameter is determined by a comparison between the residual (or discrepancy) $\|Tx_\gamma^\varepsilon - y^\varepsilon\|$ and the known noise level bound ε.

If we have the noisy data y^ε instead of y and know that $\|y - y^\varepsilon\| \leq \varepsilon$ for the operator equation $Tx = y$, it does not make sense to get an approximate solution $\tilde{x}$ with the residual $\|T\tilde{x} - y^\varepsilon\| \leq \varepsilon$ because of the fact that a smaller regularization parameter means less stability. Therefore we assume $\tau > 1$ [23].

Theorem 2.18 *([23], Theorem 4.17) The regularization method (R_γ, γ) where γ is defined via the discrepancy principle is convergent for all $y \in \mathcal{R}(T)$.*

Remark 2.19 *([23], Remark 4.18) Any parameter choice $\gamma = \gamma(\varepsilon, y^\varepsilon)$ satisfies*

$$\|Tx_\gamma^\varepsilon - y^\varepsilon\| \leq \tau\varepsilon \leq \|Tx_\beta^\varepsilon - y^\varepsilon\|$$

for some β with $\gamma \leq \beta \leq 2\gamma$, and with τ constrained by (2.20).

This is an important point for practical computations. We use this criteria as a stopping rule for outer iterative scheme in the context of Newton method. Consequently discrepancy principle defines the stopping iteration index k_* to be the first integer such that

$$\|F(x_{k_*}^\varepsilon) - y^\varepsilon\| \leq \tau\varepsilon \leq \|F(x_k^\varepsilon) - y^\varepsilon\|\,,\ 0 \leq k \leq k_*$$

for equation $\Phi(x) = y$ where $\Phi : D(\Phi) \subset X \longrightarrow Y$ is a nonlinear operator between the Hilbert spaces X and Y and $\tau > 1$ is a given number [40, 67].

2.2.3 L-Curve Method

L-Curve is an error-free parameter selection method which does not require any knowledge about the noise level ε. In this subsection we investigate the characteristics of the L-Curve parameter choice rule for Tikhonov regularization. Namely we try to find an appropriate regularization parameter for the minimization problem

$$min\left\{\|Tx - y\|_Y^2 + \gamma^2\|x\|_X^2\right\}. \tag{2.22}$$

Where we take γ^2 instead of γ as a regularization parameter because of the convenience in the numerical computations. The L-Curve is a plot of pairs $(\|Tx-y\|_Y^2, \|x\|_X^2)$ as a function of parameter γ where the pairs represent the size of the residual and the size of the solution. The L-curve has a perceptible L-shaped corner (Figure 2.2) situated exactly where the regularized solution changes from being dominated by noise to being dominated by regularization errors.

The idea of the method for choosing the regularization parameter is to determine a point on this curve that is at the corner of the vertical pieces. For this purpose

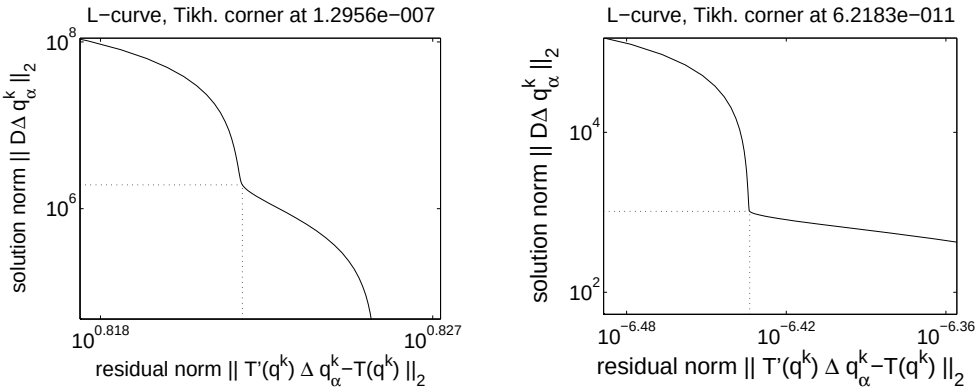

Figure 2.2: Solution norm according to residual norm with L-Curve method. Regularization parameter is on the corner of the graph after 2. iteration (left) and after 6. iteration (right).

we could choose the point on the L-Curve where the curvature is maximum. Now we want to find an efficient formula for the curvature of the L-curve. We follow the same technique as in [36] in which the curvature is given by means of singular value expansion of the operator and the Tikhonov filter function. Let $c = \|x_\gamma\|^2$ and $s = \|Tx_\gamma - y\|^2$ with x_γ be a regularized solution. From the numerical point of view it is beneficial to consider L-Curve (s, c) in a log-log scale. The behaviour of the L-Curve more easily seen in such a scale because of the several order of the magnitude of the singular values. Thus, let $\hat{c} = \log c$ and $\hat{s} = \log s$ such that L-Curve is a plot of $\hat{c}/2$ versus $\hat{s}/2$. Moreover let $\hat{c}'$, $\hat{s}'$, $\hat{c}''$ and $\hat{s}''$ denote the first and second derivatives of $\hat{c}$ and $\hat{s}$ with respect to γ. Then the curvature of the L-Curve κ is given by

$$\kappa = 2\frac{\hat{s}'\hat{c}'' - \hat{s}''\hat{c}'}{((\hat{s}')^2 + (\hat{c}')^2)^{3/2}}. \tag{2.23}$$

Here derivatives of $\hat{c}$ and $\hat{s}$ with respect to γ is defined via logarithmic differentiation, i.e.,

$$\hat{c}' = \frac{c'}{c} \text{ and } \hat{s}' = \frac{s'}{s}.$$

On the other hand, we may write the regularized solution x_γ and the corresponding residual $y - Tx_\gamma$ by using singular value expansion (σ_i, v_i, u_i) of the operator and the filter function for Tikhonov regularization as

$$x_\gamma = \sum_{i=1}^{\infty} \frac{f_i}{\sigma_i}\langle y, u_i\rangle v_i \tag{2.24}$$

$$y - Tx_\gamma = \sum_{i=1}^{\infty}(1 - f_i)\langle y, u_i\rangle u_i. \tag{2.25}$$

where f_i is defined by

$$f_i := \frac{\sigma_i^2}{\sigma_i^2 + \gamma^2} \tag{2.26}$$

such that the term $\frac{f_i}{\sigma_i}$ gives the filter function for Tikhonov regularization. From (2.24) and (2.25) we may write

$$c = \|x_\gamma\|^2 = \sum_{i=1}^{\infty} \left(\frac{f_i}{\sigma_i} \langle y, u_i \rangle \right)^2 \tag{2.27}$$

$$s = \|y - T x_\gamma\| = \sum_{i=1}^{\infty} \left((1 - f_i) \langle y, u_i \rangle \right)^2 . \tag{2.28}$$

Furthermore by using the derivatives

$$\frac{\mathrm{d} f_i^2}{\mathrm{d}\gamma} = -\frac{4}{\gamma}(1 - f_i) f_i^2, \quad \frac{\mathrm{d}(1 - f_i)^2}{\mathrm{d}\gamma} = \frac{4}{\gamma}(1 - f_i)^2 f_i$$

we get the derivatives of c and s with respect γ as follows:

$$c' = \sum_{i=1}^{\infty} -\frac{4}{\gamma}(1 - f_i) f_i^2 \frac{\beta_i^2}{\sigma_i^2} \tag{2.29}$$

$$s' = \sum_{i=1}^{\infty} \frac{4}{\gamma}(1 - f_i)^2 f_i \beta_i^2 \tag{2.30}$$

where $\beta_i = \langle y, u_i \rangle$. Now on using

$$\frac{f_i}{\sigma_i^2} = \frac{1}{\sigma_i^2 + \gamma_i^2} = \frac{1 - f_i}{\gamma_i^2}$$

we obtain the relation between s' and c' as $s' = -\gamma^2 c'$. The second derivatives of $\hat{c}$ and $\hat{s}$ with respect to γ are given by

$$\hat{c}'' = \frac{\mathrm{d}}{\mathrm{d}\gamma}\frac{c'}{c} = \frac{c''c - (c')^2}{c^2} \quad \textit{and} \quad \hat{s}'' = \frac{\mathrm{d}}{\mathrm{d}\gamma}\frac{s'}{s} = \frac{s''s - (s')^2}{s^2}.$$

Additionally we have

$$s'' = \frac{\mathrm{d}}{\mathrm{d}\gamma}(-\gamma^2 c') = -2\gamma c' - \gamma^2 c''.$$

Finally if we insert all expressions for $\hat{c}'$, $\hat{c}''$, $\hat{s}'$ and $\hat{s}''$ into (2.23) we reach the following formula for curvature κ.

$$\kappa = 2\frac{cs}{c'} \frac{\gamma^2 c' s + 2\gamma c s + \gamma^4 c c'}{(\gamma^2 c^2 + s^2)^(3/2)}$$

in which the quantities c, s and c' are given in (2.27), (2.28) and (2.29) respectively.

2.2.4 Generalized Cross Validation (GCV)

Generalized cross validation is proposed in [30] as a parameter choice rule which works without any prior information about the noise level ε. This method selects the regularization parameter γ which minimizes the functional

$$G(\gamma) = \frac{n\|Tx_\gamma - y\|_2^2}{trace(I - T_\gamma)} \tag{2.31}$$

where $T_\gamma = T(T^*T + \gamma L)^{-1}T^*$ is an n by n matrix for Tikhonov regularization. The computation of the defined functional can be done with the generalized singular value expansion $(\hat{\sigma_j}, \hat{v}_j, \hat{u}_j)_{j\in\mathbb{N}}$ of the operator T and L [78]. Indeed the functional in (2.31) will be

$$G(\gamma) = \frac{n\sum_{\sigma_i>0}(f_i - 1)^2\beta_i^2 + n\sum_{\sigma_i=0}\beta_i^2}{[n - \sum_{\sigma_i>0} f_i]^2} \tag{2.32}$$

in which f_i is given in (2.26) and $\beta_i = \hat{u}_i^T y$.

2.3 Ill-Posed Nonlinear Operator Equations

Unlike the linear case, ill-posed problems from nonlinear operators are not well developed. This makes the nonlinear ill-posed problems the area of growing interest in the applied sciences. In this section we deal with the equation

$$\Phi(x) = y \tag{2.33}$$

where $\Phi : D(\Phi) \subset X \longrightarrow Y$ is a nonlinear operator between the Hilbert spaces X and Y. When we consider the ill-posedness of nonlinear operator we always mean that the solutions do not depend continuously on the data. In the nonlinear case the operator Φ has the following properties.

(i) Φ is continuous.

(ii) Φ is weakly closed, i.e., for any sequence $\{x_n\} \subset D(\Phi)$, weak convergence of x_n to x in X and weak convergence of $\Phi(x_n)$ to y in Y imply that $x \in D(\Phi)$ and $\Phi(x) = y$.

In the linear case we looked for the minimum-norm solution. But for nonlinear operator we search for the x_0-minimum norm solution $x^\dagger$, i.e.,

$$\Phi(x^\dagger) = y$$

and

$$||x^\dagger - x_0|| = min\{||x - x_0|| \mid \Phi(x) = y\}.$$

This choices cause from the fact that a solution of a nonlinear problem may not be unique. Therefore the choices of x_0 will be very important, especially for the local results about convergence. Available a-prior information about the solution of course have an impact on the selection of the x_0.

2.3.1 Iterative Methods For Nonlinear Equations

Let us consider a nonlinear operator $\Phi : D(\Phi) \subset X \longrightarrow Y$ where X and Y are Hilbert spaces. We denote

$$\Omega_R(x_0) = \{x \in X \mid ||x - x_0||_X \leq R\}\ ,\ x_0 \in X$$

and suppose $\Phi(x)$ is Frechet differentiable on $\Omega_R(x_0)$ with the Lipschitz continuous derivative $\Phi'(x)$ so that

$$||\Phi'(x_1) - \Phi'(x_2)||_Y \leq L||x_1 - x_2||_X\ ,\ L \in \mathbb{R}.$$

Now we aim to find a solution to an equation

$$\Phi(x) = y\ ,\ x \in \Omega_R(x_0) \tag{2.34}$$

near the point $x_0 \in X$. Let x^* be a solution of (2.34). With the help of the linearization formula around x_0 we have

$$\Phi(x_0) - y + \Phi'(x_0)(x^* - x_0) = 0. \tag{2.35}$$

If we assume the operator $\Phi'^*(x_0)\Phi'(x_0) : X \longrightarrow X$, where "*" denotes the adjoint operator, has a continuous inverse then (2.34) is a regular equation and the approximate solution of the normal equation $\Phi'^*(x_0)\Phi'(x_0)(x^* - x_0) = \Phi'^*(x_0)(y - \Phi(x_0))$

$$x^* \approx x_0 + (\Phi'^*(x_0)\Phi'(x_0))^{-1}\Phi'^*(x_0)(y - \Phi(x_0)) \tag{2.36}$$

can be found from the well-posed least square problem related to (2.35):

$$min\left\{\|\Phi(x_0) - y + \Phi'(x_0)(x^* - x_0)\|_Y^2 \mid (x^* - x_0) \in X\right\}. \tag{2.37}$$

If the problem (2.37) is ill-posed, the approximation in (2.36) loses its meaning because of the compactness of $\Phi'(x_0)$ which comes from the continuity and compactness of $\Phi(x_0)$ [12, 23].

It is well-known that iteration of (2.36) provides a foundation for construction of rapidly converging numerical methods for regular type of (2.34). In this manner Gauss-Newton Method will be obtained as

$$x_{n+1} = x_n + (\Phi'^*(x_n)\Phi'(x_n))^{-1}\Phi'^*(x_n)(y - \Phi(x_n)) \ , \ n = 0, 1, \dots . \tag{2.38}$$

Local convergence of (2.38) is guaranteed by the continuity of $\Phi'^*(x_n)\Phi'(x_n)$ and the condition $x \in \Omega_R(x_0)$. However, in the ill-posed case, (2.38) does not produce a solution, and to obtain reasonable approximate solution some sort of regularization will be necessary.

2.3.2 Regularization of Nonlinear Ill-posed Problems

The standard form of the Newton-type methods for solving nonlinear equation (2.33) can be obtained by means of the linearized version of (2.33) at a current iterate x_n as

$$\Phi'(x_n)(x - x_n) = y - \Phi(x_n). \tag{2.39}$$

For inverse problems the inverse of $\Phi'^*(x)\Phi'(x)$ is unbounded. This causes unstable iteration processes. To overcome this difficulty the term $(\Phi'^*(x)\Phi'(x))^{-1}$ need to be replaced by a bounded operator, i.e., a regularization operator. If we apply Tikhonov regularization to (2.39) we obtain the most common iterative method for nonlinear ill-posed equation, namely Levenberg-Marquardt method:

$$x_{n+1} = x_n + (\Phi'^*(x_n)\Phi'(x_n) + \gamma_n I)^{-1}\Phi'^*(x_n)(y^\varepsilon - \Phi(x_n)). \tag{2.40}$$

Where γ_n be a sequence of regularization parameters and y^ε be the noisy right hand side of (2.34) with a known or unknown noise level ε.

Another method proposed by Bakushinsky [11] known as iteratively regularized Gauss-Newton method:

$$x_{n+1} = x_n + (\Phi'^*(x_n)\Phi'(x_n) + \gamma_n I)^{-1}\Phi'^*(x_n)(y^\varepsilon - \Phi(x_n) + \gamma_n(x_n - x_0)). \tag{2.41}$$

Actually both updates can be considered as a solution of Tikhonov minimization problem

$$\|\Phi(x) - y^\varepsilon\|^2 + \gamma_n\|x - x^1\|^2 = min! \tag{2.42}$$

with Φ linearized around x_n:

$$\|\Phi(x_n) + \Phi'(x_n)(x_{n+1}^{LM} - x_n) - y^\varepsilon\|^2 + \gamma_n\|x_{n+1}^{LM} - x_n\|^2 = min! \tag{2.43}$$

$$\|\Phi(x_n) + \Phi'(x_n)(x_{n+1}^{GN} - x_n) - y^\varepsilon\|^2 + \gamma_n\|x_{n+1}^{GN} - x_0\|^2 = min! \tag{2.44}$$

In the Levenberg-Marguardt method (2.43) a priori estimate x^1 in the regularizing term $\|x - x^1\|$ is the last iterate and changes in each iteration. On the other hand it is fixed as x_0 in the second method (2.44). Therefore the additional term $(\Phi'^*(x_n)\Phi'(x_n)+ \gamma_n I)^{-1}\gamma_n(x_n - x_0)$ is the only difference between two methods and it has a stability effect [11]. Convergence properties of both methods has been investigated by several authors [11, 12, 14, 34] in details.

CHAPTER 3

SINGULAR INVERSE STURM LIOUVILE PROBLEM OVER $(-\infty, \infty)$

Here, in this chapter the problem is regarded as singular when it is defined on an infinite interval of x, $x \in (-\infty, \infty)$, i.e., we do not suppose any integrability property of $|q|$ over $(-\infty, \infty)$ so that the singular problem cannot be transformed to a regular problem on a finite interval [58]. We deal with the canonical form of the singular Sturm-Liouville (S-L) problem

$$-y'' + q(x)y = \lambda y, \quad x \in (-\infty, \infty). \tag{3.1}$$

We assume that all functions are real-valued and continuous. We are looking for solutions of class $L^2(-\infty, \infty)$ and we are interested in problems of limit-point type. That is, if (3.1) has a nontrivial solution $y \in L^2(-\infty, \infty)$ then λ must be an eigenvalue and y the corresponding eigenfunction. Therefore, no boundary conditions are needed at infinity [20]. We only regard potential functions $q(x)$ which are bounded from below. This means, the problem has a finite or enumerable infinite number of discrete eigenvalues with $+\infty$ as the only accumulation point.

There are several methods to calculate the eigenvalues and eigenfunctions of singular S-L problem on the real line for a given potential function $q(x)$. We can roughly divide these methods into two different types by keeping in mind the literature. The first one is domain truncation, i.e., approximation of the singular S-L problem by a regular S-L problem over a finite interval $x \in [-l, l]$ with l sufficiently large [10, 63, 65, 73, 79]. The second type of methods depend on the series expansion of the solution via basis functions intrinsic to an infinite interval, such as Hermite polynomials or sinc-functions [16, 74]. Both approaches reduce the problem to a matrix-eigenvalue

problem.

On the other hand inverse problems have much more difficulties in comparing with the direct problem. As an inverse problem, as regarded here, the question is to determine the potential function q from eigenvalues, notably the celebrated works by Borg [15] and by Gel'fand and Levitan [28] in which the fundamental fact that two sets of data sequences are required to uniquely determine a potential are settled. A quick introduction to regular inverse S-L problem can be found in Chadan et al. [19]. One type is based on simple matrix methods. Recently, for the first time a numerical method based on Numerov's method was proposed by Andrew [3] to estimate the potential q from eigenvalues which uses asymptotic correction with a fourth-order method and offers significant advantages. Another type consists in transforming the regular S-L problem to a hyperbolic Cauchy or Goursat problem [66, 69]. A further type constructs particularly sui functionals which one has to minimize in recovering the potential [17, 68]. However, the recovery of a potential from spectral data is a difficult and ill-conditioned numerical problem.

In this chapter we present for the first time to our knowledge a recovery method for singular inverse S-L problem by using regularization techniques.

3.1 Numerical Preliminaries

In the following sections the potential q is assumed additionally to be symmetric

$$q(x) = q(-x), \tag{3.2}$$

i.e., one needs only one sequence of eigenvalues to recover the potential. Therefore, let us define our singular inverse S-L problem in the numerical "finite" sense: For the given first n eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$ of (3.1) in which the potential q satisfies the symmetry condition (3.2), we want to find a vector which represents the values of the potential at certain nodes. In this procedure one faces with some difficulties. First of all, our singular inverse problem has an ill-conditioned structure. Because of that reason regularization techniques are needed. Secondly, since the numerical implementation will end with a non-linear equation, an iteration procedures is necessary in this case, such as Newton's method. This yields the determination of a suitable

initial guess and the Jacobian matrix in each iteration step as accurate and stable as possible. Thirdly, we have to approximate the eigenvalues as accurate as possible for the supplied potential in each iteration step by a direct methods. In addition to these difficulties we have some parameters, such as the domain truncation parameter l and the number of used eigenvalues, which has to be estimated. Unfortunately, the determination of these parameters suitably depends on the solution procedure in a strict way.

3.1.1 Pseudospectral Method for Direct Problems

If one wants to solve the problem (3.1) it is necessary to approximate the second derivative of y. It should be done via finite difference methods, Rayleigh-Ritz method or pseudospectral (spectral collocation) methods. In the last method, the derivation of the differentiation matrices depends basically on interpolation. In connection with this we consider the weighted interpolants of the form

$$y(x) \approx P_{N-1}(x) = \sum_{j=1}^{N} \frac{\beta(x)}{\beta(x_j)} \phi_j(x) y_j \tag{3.3}$$

in which $\left\{x_j\right\}_{j=1}^{N}$ is the set of distinct interpolation nodes, $\beta(x)$ is a weight function, $y_j = y(x_j)$, and $\left\{\phi_j(x)\right\}_{j=1}^{N}$ are interpolating basis functions satisfying $\phi_j(x_k) = \delta_{jk}$ with Kronecker's delta δ_{jk}. It is easy to see $y(x_k) = P_{N-1}(x_k)$ for $k = 1, \ldots, N$. Here, if the nodes are taken as N roots of orthogonal polynomials, such as Chebyshev, Hermite, Laguerre, P_{N-1} will be a polynomial of $(N-1)$st degree. On the other hand there are two well-known non-polynomial cases, namely trigonometric (Fourier) and sinc (cardinal) interpolants. Here, in this subsection we will interested in the trigonometric case.

We may approximate the derivative function y' by taking the derivative of (3.3) and evaluating it at the nodes x_k, i.e.,

$$y'(x_k) \approx P'_{N-1}(x_k) = \sum_{j=1}^{N} \frac{\mathrm{d}}{\mathrm{d}x} \left[\frac{\beta(x)}{\beta(x_j)} \phi_j(x)\right]\Bigg|_{x=x_k} y_j, \qquad k = 1, \ldots, N.$$

It gives a system which should be correspond to the differentiation matrix

$$\boldsymbol{D}^{(1)}_{k,j} := \frac{\mathrm{d}}{\mathrm{d}x} \left[\frac{\beta(x)}{\beta(x_j)} \phi_j(x)\right]\Bigg|_{x=x_k}, \qquad j,k = 1, \ldots, N. \tag{3.4}$$

Depending on this representation the numerical derivative of y can be written in a matrix-vector product

$$\boldsymbol{y}^{(1)} = \boldsymbol{D}^{(1)}\boldsymbol{y}, \tag{3.5}$$

in which $\boldsymbol{y}^{(1)}$ and $\boldsymbol{y}$ are the vectors of approximate derivative values and function values at the grid points, respectively. By the same way it is possible to derive further derivatives of the function $y(x)$ at the grid points in a matrix-vector product form. For our S-L problem it is enough to calculate the second derivative.

3.1.2 Pseudospectral Method in the Non-Polynomial Case

In the trigonometric (Fourier) case, bounded and periodic grids on the interval $[0, 2\pi]$ are assumed. In other words nodes are chosen in the following way

$$x_k = kh, \quad h = \frac{2\pi}{N}, \quad k = 1, \ldots, N-1.$$

And the interpolant in (3.3) is written as

$$T(x) = \sum_{j=1}^{N-1} \phi_j(x) y_j$$

by selecting the weight function $\beta(x) = 1$ and the interpolation functions

$$\phi_j(x) = \frac{h}{2\pi} \sin[\frac{\pi}{h}(x - x_j)] \cot[\tfrac{1}{2}(x - x_j)], \quad k = 1, \ldots, N-1. \tag{3.6}$$

Taking the derivative of (3.6) and putting $x = x_k$ we have by using the definition of grid points

$$\phi_j'(x_k) = \frac{1}{2}\left\{\cos[\pi(k-j)] \cot[\tfrac{1}{2}(k-j)h] - \frac{h}{\pi} \sin[\pi(k-j)] \csc^2[\tfrac{1}{2}(k-j)h]\right\}$$

for $k, j = 1, \ldots, N-1$.

Now by using this derivatives at $x = x_k$ the first order differentiation matrix is in the form

$$\boldsymbol{D}^{(1)}_{k,j} = \left[\frac{\mathrm{d}}{\mathrm{d}x}\phi_j(x)\right]\Big|_{x=x_k} = \begin{cases} 0 & \text{if} \quad k = j \\ \frac{1}{2}(-1)^{k-j} \cot[\frac{1}{2}(k-j)h] & \text{if} \quad k \neq j \end{cases}$$

for $j, k = 1, \ldots, N-1$.

In a similar fashion the second order derivative values at the grid points lead to the result

$$\boldsymbol{D}^{(2)}_{k,j} = -\frac{1}{6}\begin{cases} \dfrac{2\pi^2}{h^2}+1 & \text{if} \quad k=j \\ \frac{1}{2}(-1)^{k-j}\csc^2[\frac{1}{2}(k-j)h] & \text{if} \quad k\neq j \end{cases}, \qquad j,k=1,\ldots,N-1 \tag{3.7}$$

for the elements of the second order differentiation matrix $D^{(2)}$, see e.g. [79].

On the other hand, when we want to apply this method to our problem (3.1) we have to truncate our infinite interval to $[-l, l]$. After this, with a basic transformation

$$\hat{x} = \frac{1}{\pi}(x-\pi)l$$

we carry all grid points from $[0, 2\pi]$ to $[-l, l]$. Here, since we take all grids in the interior, it should be assumed that Dirichlet boundary conditions $y(l) = y(-l) = 0$ taken into account according to truncated problem. And because of the transformation our second order differentiation matrix in (3.7) has to be multiplied by $(\frac{\pi}{l})^2$. Actually we have

$$\frac{\mathrm{d}^2y}{\mathrm{d}\hat{x}^2} = (\frac{\pi}{l})^2\frac{\mathrm{d}^2y}{\mathrm{d}x^2}, \quad \hat{x}\in[-l,l], \quad x\in[0,2\pi].$$

Now we can write the direct S-L problem (3.1) in a matrix-eigenvalue form by using pseudospectral differentiation

$$(\,\boldsymbol{D}^{(2)}_{N-1} + \boldsymbol{Q}\,)\boldsymbol{y} = \Lambda\boldsymbol{y} \tag{3.8}$$

in which $\boldsymbol{D}^{(2)}_{N-1}$ is the second order differentiation matrix in (3.7) multiplied by the factor $(\frac{\pi}{l})^2$ and $\boldsymbol{Q}$ is a diagonal matrix containing the values of the potential at grid points in its diagonal entries. It is easy to see that both matrices are symmetric and they are $(N-1)$-dimensionally square matrices.

3.1.3 Pseudospectral Method in Polynomial Case (Hermite Pseudospectral Method)

In this subsection we give a summary for the Hermite Pseudospectral Method following from the paper [74]. The polynomial interpolation based on the Lagrange interpolation is the key point for the formulation of the differentiation matrices for the pseudospectral method in the polynomial case. Thus, before formulating the Hermite Pseudospectral Method we briefly mention about the polynomial interpolation.

Afterwards we touch the relation between Hermite Pseudospectral Method and Lagrange polynomial interpolation. First of all since we study with an infinite domain in our problem, we consider the scaled variable t,

$$t = \alpha x, \qquad \alpha > 0 \tag{3.9}$$

instead of original variable x in (3.1). The transformation in (3.9) transforms our problem (3.1) into the form

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \frac{1}{\alpha^2} q\left(\frac{t}{\alpha}\right)\right] y(t) = \mathcal{E}(\alpha) y(t), \qquad y \in L_2(-\infty, \infty). \tag{3.10}$$

Where the eigenvalues $\mathcal{E}(\alpha)$ of (3.10) are linked with the eigenvalues λ of the original equation (3.1) by the relation

$$\lambda = \alpha^2 \mathcal{E}(\alpha). \tag{3.11}$$

Here the optimization parameter α plays an important role in the numerical treatment.

Now, in relation to polynomial interpolation let us consider the so-called Lagrange polynomials of Nth degree of the form

$$\ell_k(t) = \frac{\pi(t)}{(t - t_k)\pi'(t_k)}, \qquad k = 0, 1, \ldots \tag{3.12}$$

in which

$$\pi(t) = \prod_{j=0}^{N} (t - t_j) \tag{3.13}$$

represents a polynomial of degree $N + 1$ and $t_0 < t_1 < \ldots < t_N$ are distinct roots of $\pi(t)$. The Lagrange polynomial set $\{\ell_k(t)\}$ has the well-known property $\ell_k(t_j) = \delta_{jk}$ where δ_{jk} is the Kronecker's delta. Then, it is possible to approximate any function $g(t)$ uniquely by the Lagrange interpolation formula of the form

$$P(t) = \sum_{k=0}^{N} \ell_k(t) g_k, \qquad g(t) = P(t) + R_N(t) \tag{3.14}$$

in which $g_k = g(t_k)$. Here (3.14) represents a polynomial, having the possible lowest degree N, satisfying $P(t_k) = g_k,\ n = 0, 1, \ldots, N$ which allows us to vanish the error term $R_N(t)$ at the nodes $t = t_k$. Moreover, if $g(t)$ is also a polynomial of degree N, then Lagrange interpolation $P(t)$ would be considered as an alternative exact representation of $g(t)$.

On the other hand if we differentiate the expressions for $P(t)$ and $g(t)$ in (3.14) we reach the derivative of the polynomial, i.e., $P'(t)$ and the approximation of the derivative of the function, namely $g'(t)$ in the form

$$P'(t) = \sum_{k=0}^{N} \ell'_k(t) g_k, \qquad g'(t) = P'(t) + R'_N(t). \tag{3.15}$$

Moreover, it is possible to determine the derivative values at $N+1$ nodes $\{t_k\}$ with the help of $g_k = P(t_k)$ with a differentiation matrix defined by

$$\boldsymbol{D}^{(1)} := [d_{jk}^{(1)}] = [\ell'_k(t_j)] \tag{3.16}$$

for $j, k = 0, 1, \ldots, N$. Indeed we have

$$P'(t_j) = \sum_{k=0}^{N} \ell'_k(t_j) g_k = \sum_{k=0}^{N} d_{jk}^{(1)} P(t_k), \qquad j = 0, 1, \ldots, N \tag{3.17}$$

which can be converted in the following matrix-vector form

$$\boldsymbol{g}^{(1)} = \boldsymbol{D}^{(1)} \boldsymbol{g}, \tag{3.18}$$

Here $\boldsymbol{g}^{(1)} = [P'(t_0), P'(t_1), \ldots, P'(t_N)]^{\mathrm{T}}$ and $\boldsymbol{g} = [P(t_0), P(t_1), \ldots, P(t_N)]^{\mathrm{T}}$. The elements $d_{jk}^{(1)}$ of the first order differentiation matrix $\boldsymbol{D}^{(1)}$ can be obtained explicitly from the definition of the Lagrange polynomials in (3.12) as

$$d_{jk}^{(1)} = \begin{cases} \dfrac{\pi'(t_j)}{(t_j - t_k)\pi'(t_k)} & \text{if } j \neq k \\ \dfrac{\pi''(t_k)}{2\,\pi'(t_k)} & \text{if } j = k \end{cases} \tag{3.19}$$

in which $j, k = 0, 1, \ldots, N$.

In a similar way the second order differentiation matrix $\boldsymbol{D}^{(2)} := [d_{jk}^{(2)}]$ can be derived with its entries

$$d_{jk}^{(2)} = \begin{cases} \dfrac{1}{t_j - t_k}\left[\dfrac{\pi''(t_j)}{\pi'(t_k)} - 2d_{jk}^{(1)}\right] & \text{if } j \neq k \\ \dfrac{\pi'''(t_k)}{3\,\pi'(t_k)} & \text{if } j = k \end{cases} \tag{3.20}$$

comes from the relation with the Lagrange polynomials $d_{jk}^{(2)} = \ell''_k(t_j)$. And using this expression, the second derivative values may be written in the same form with (3.18) as

$$\boldsymbol{g}^{(2)} = \boldsymbol{D}^{(2)} \boldsymbol{g} \tag{3.21}$$

where $\boldsymbol{g}^{(2)} = [P''(t_0), P''(t_1), \ldots, P''(t_N)]^{\mathrm{T}}$ is a vector containing the second derivative values at nodes.

The derivation of the higher order differentiation matrix can be found in [80]. But the differentiation matrices up to second order are sufficient for our second order problem.

At this moment we are able to attain the matrix representation of the Sturm-Liouville equation with the help of differentiation matrices. Now, we transform the equation (3.10) to

$$-u'' + 2tu' + V(t)u = (\mathcal{E}(\alpha) - 1)u \tag{3.22}$$

by defining

$$y(t) = \mathrm{e}^{-t^2/2}u(t), \tag{3.23}$$

to factor out the weight $\mathrm{e}^{-t^2/2}$ for Hermite polynomials. Here $u(t)$ is the new dependent variable and

$$V(t) = \frac{1}{\alpha^2}q\left(\frac{t}{\alpha}\right) - t^2 \tag{3.24}$$

is regarded as the modified potential. Let

$$\phi_k(t) = \frac{1}{\sqrt{2^k k!\,\sqrt{\pi}}}\,H_k(t), \qquad k = 0, 1, \ldots \tag{3.25}$$

represent the normalized Hermite polynomials in which $H_k(t)$ are the classical Hermite polynomials. With this statement the usual three-term recurrence relation $H_{k+1} = 2tH_k - 2kH_{k-1}$ of the classical Hermite polynomials takes the form

$$\sqrt{k}\phi_{k-1}(t) - \sqrt{2}t\phi_k(t) + \sqrt{k+1}\phi_{k+1}(t) = 0, \quad k = 0, 1, \ldots, N, \ldots \tag{3.26}$$

where $\phi_{-1}(t) = 0$ and $\phi_0(t) = \pi^{-1/4}$. Now let us propose the trial solution for the equation (3.22) of the type

$$u_{\mathrm{T}}(t) = \sum_{k=0}^{N} u_k \ell_k(t) \tag{3.27}$$

proposed by the Lagrange interpolation formula in (3.14), where

$$\ell_k(t) = \frac{\phi_{N+1}(t)}{(t - t_k)\phi'_{N+1}(t_k)} = \frac{H_{N+1}(t)}{(t - t_k)H'_{N+1}(t_k)}, \quad k = 0, 1, \ldots, N \tag{3.28}$$

are the Lagrange polynomials. Thus, we require the real and distinct roots of $\phi_{N+1}(t)$ or $H_{N+1}(t)$ as a collocation points for the interpolation. Actually we will take

$$\pi(t) = \phi_{N+1}(t) \quad \text{and} \quad \phi_{N+1}(t_j) = 0 \tag{3.29}$$

related with (3.13). The roots of H_{N+1} can be obtained from the recursion in (3.26). Namely if we write the first $N+1$ equations of (3.26) we arrive at the inhomogeneous linear system

$$\begin{bmatrix} -\sqrt{2}t & \sqrt{1} & 0 & \cdots & 0 \\ \sqrt{1} & -\sqrt{2}t & \sqrt{2} & \ddots & \vdots \\ 0 & \sqrt{2} & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & -\sqrt{2}t & \sqrt{N} \\ 0 & \cdots & 0 & \sqrt{N} & -\sqrt{2}t \end{bmatrix} \begin{bmatrix} \phi_0(t) \\ \phi_1(t) \\ \vdots \\ \phi_{N-1}(t) \\ \phi_N(t) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ -\sqrt{N+1}\,\phi_{N+1}(t) \end{bmatrix}. \quad (3.30)$$

If we choose the last element of the right hand side is zero, i.e., $\phi_{N+1}(t) = 0$, we meet with the standart matrix eigenvalue problem $\boldsymbol{R}\boldsymbol{z} = t\boldsymbol{z}$ where $\boldsymbol{R}$ is a symmetric tridiagonal matrix

$$\boldsymbol{R} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & \sqrt{1} & 0 & \cdots & 0 \\ \sqrt{1} & 0 & \sqrt{2} & \ddots & \vdots \\ 0 & \sqrt{2} & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & \sqrt{N} \\ 0 & \cdots & 0 & \sqrt{N} & 0 \end{bmatrix} \quad (3.31)$$

whose eigenvalues t_j are the desired roots of $H_{N+1}(t)$ for $j = 0, 1, \ldots, N$. Now if we substitute (3.26) into (3.22) and enforce it to satisfy at the nodes $t_0, t_1, \ldots, t_N$ we obtain the algebraic equations

$$\sum_{k=0}^{N} \left[-\ell_k''(t_j) + 2t_j \ell_k'(t_j) + V_j \ell_k(t_j) \right] u_k = (\mathcal{E}(\alpha) - 1) \sum_{k=0}^{N} \ell_k(t_j) u_k \quad (3.32)$$

for $j = 0, 1, \ldots, N$. At this point we are able to write (3.32) as a matrix representation of the equation (3.22)

$$(\boldsymbol{\mathcal{B}} + \boldsymbol{V})u = (\mathcal{E}(\alpha) - 1)u \quad (3.33)$$

where the general entry B_{jk} of $\boldsymbol{\mathcal{B}}$ is given by

$$B_{jk} = -d_{jk}^{(2)} + 2t_j d_{jk}^{(1)} \quad (3.34)$$

and the entries V_j of the modified potential V are defined by $V_j := V(t_j)$. In this picture $d_{jk}^{(1)}$ and $d_{jk}^{(2)}$ are given in (3.19) and (3.20) respectively with defined $\pi(t)$ in (3.29). Thus, imposing (3.29) into (3.19) and (3.20) it is possible to write down the

elements of B_{jk},

$$B_{jk} = \begin{cases} \dfrac{2}{(t_j - t_k)^2} & \text{if } j \neq k \\ \\ \dfrac{2}{3(N + t_k^2)} & \text{if } j = k. \end{cases} \tag{3.35}$$

It can be easily seen that $B_{jk} = B_{kj}$, i.e., $\mathcal{B}$ is a symmetric matrix. Thus, we have the symmetric eigenvalue problem

$$(B_{jk} + V_j \delta_{jk})u = (\mathcal{E}(\alpha) - 1)u \tag{3.36}$$

with an eigenvalues $(\mathcal{E}(\alpha)-1)$. This symmetric eigenvalue problem helps us to recover the modified potential $V(t)$ from the given eigenvalues $(\mathcal{E}(\alpha) - 1)$ related with the formula (3.11).

3.2 Development of the Inverse Problem

For the given first n eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$ of (3.1) with the information $q(x) = q(-x)$ about the potential, the inverse problem is concerned to find an n-vector whose components give an approximation to $q_i = q(ih)$, $i = 1, \ldots, n$, where $h = \frac{2l}{2n+1}$ with the truncation parameter l. During the solution process we consider this problem as a nonlinear equation in the form

$$\boldsymbol{T}(q) = 0 \tag{3.37}$$

where the ith component t_i of the vector $\boldsymbol{T}(q)$ carries the difference

$$t_i(q_1, \ldots, q_n) = \Lambda_i(q_1, \ldots, q_n) - (\lambda_i^{\text{sing}})^{\delta}, \quad i = 1, \ldots, n \tag{3.38}$$

in which $\{\Lambda_i\}_{i=1}^n$ is the set of approximated eigenvalues of (3.1) corresponding to the truncated problem with step length h and $q(ih)$. It is possible to solve this nonlinear equation system with an iterative method. This means we give an initial potential q^0 and calculate the eigenvalues $\Lambda_i^{(0)}$ of (3.1). Then we compare this set with the given eigenvalue set $(\lambda_i^{\text{sing}})^{\delta}$ for $i = 1, \ldots, n$. The index δ is the noise level which describes the differing asymptotic behaviour of the given differential eigenvalues and the required finite difference eigenvalues after discretization as a well-known fact and, if necessary, additionally the accuracy of the given singular eigenvalues. Other

methods for regular inverse S-L problem deal with an algebraic correction, see e.g. [3, 59]. Then one continues the iteration process until the difference $\Lambda_i^{(k)} - (\lambda_i^{\text{sing}})^\delta$ is small enough with respect to the noise level δ, roughly spoken. Here k denotes the iteration number. In that picture Newton's method may be formulated as

$$\boldsymbol{q}^{k+1} = \boldsymbol{q}^k - (\boldsymbol{T}'(\boldsymbol{q}^k))^{-1}\boldsymbol{T}(\boldsymbol{q}^k) \tag{3.39}$$

where $\boldsymbol{T}'(q^k)$ is a Jacobian matrix of type (n, n) whose computation will be visited and the ith component of $\boldsymbol{T}(\boldsymbol{q}^k)$ is $\Lambda_i^k - (\lambda_i^{\text{sing}})^\delta$, in which Λ_i^k is the ith eigenvalue of

$$\boldsymbol{\mathcal{H}}\boldsymbol{y}^k = \boldsymbol{\Lambda}\boldsymbol{y}^k \tag{3.40}$$

for $i = 1, \ldots, n$. In view of the pseudospectral methods we have two different $\boldsymbol{\mathcal{H}}$ matrix. One comes from the non-polynomial case, of the form $(-\boldsymbol{D}_{2n}^{(2)} + \boldsymbol{Q})$ leading to the matrix eigenvalue problem

$$(-\boldsymbol{D}_{2n}^{(2)} + \boldsymbol{Q}^k)\boldsymbol{y}^k = \Lambda\boldsymbol{y}^k \tag{3.41}$$

for $i = 1, \ldots, n$. In (3.41), $\boldsymbol{D}_{2n}^{(2)}$ is the second order pseudospectral differentiation matrix (3.7) but of type $(2n, 2n)$, $\boldsymbol{Q}^k$ is the diagonal matrix of type $(2n, 2n)$ with diagonal entries $(q_1^k, q_2^k, \ldots, q_n^k, q_n^k, \ldots, q_1^k)$ with the definitions $q_i^k := q^k(ih)$.The second choices of $\boldsymbol{\mathcal{H}}$ is related with the Hermite pseudospectral method. In this method we have some modifications. Actually we recover the modified potential V instead of the original potential q. In this picture we have $\boldsymbol{\mathcal{H}} = \boldsymbol{\mathcal{B}} + \boldsymbol{V}$ in which $\boldsymbol{\mathcal{B}}$ and $\boldsymbol{V}$ are square matrices with dimensions $2n$. The entries of $\boldsymbol{\mathcal{B}}$ are given in (3.35) and $\boldsymbol{V}$ is a diagonal matrix with entries carrying the value of the modified potential $V(\xi)$ at the nodes which are the roots of Hermite polynomials of degree $2n$. Thus, we have the matrix eigenvalue problem

$$(\boldsymbol{\mathcal{B}} + \boldsymbol{V}^k)\boldsymbol{u}^k = \boldsymbol{\Lambda}\boldsymbol{u}^k \tag{3.42}$$

in which $\boldsymbol{\Lambda} = (\mathcal{E}(\alpha) - 1)$.

Now if we rewrite the relation (3.39) as

$$\boldsymbol{T}'(\boldsymbol{q}^k)[\boldsymbol{q}^{k+1} - \boldsymbol{q}^k] = -\boldsymbol{T}(\boldsymbol{q}^k)$$

and in defining $\Delta\boldsymbol{q}^k = \boldsymbol{q}^{k+1} - \boldsymbol{q}^k$ which is the common "Newton's correction" we have the following equation

$$\boldsymbol{T}'(q^k)\Delta\boldsymbol{q}^k = -\boldsymbol{T}(\boldsymbol{q}^k). \tag{3.43}$$

After solving this for Newton's correction $\Delta \boldsymbol{q}^k$, we modify the solution in each iteration by

$$\boldsymbol{q}^{k+1} = \boldsymbol{q}^k + \Delta \boldsymbol{q}^k. \tag{3.44}$$

3.2.1 Computation of the Jacobian Matrix

Actually the (i, j)th element of the Jacobian matrix is the partial derivative of Λ_i with respect to the jth diagonal element of $\boldsymbol{Q}^k$, namely $\dfrac{\partial \Lambda_i}{\partial q_j}$. Now let $\boldsymbol{T}'(\boldsymbol{q}^k) := \Lambda_{i,j}$ in which the , j subscript represents the partial derivative mentioned above. Our technique to compute $\Lambda_{i,j}$ is similar to [5, 6, 24]. For this task we differentiate (3.41) and (3.42) with respect to q_j, whenever all the partial derivatives exist, i.e.,

$$-\boldsymbol{D}_{2n}^{(2)} \boldsymbol{y}_{i,j}^k + \boldsymbol{Q}_{,j}^k \boldsymbol{y}_i^k + \boldsymbol{Q}^k \boldsymbol{y}_{i,j}^k = \Lambda_{i,j}^k \boldsymbol{y}_i^k + \Lambda_i^k \boldsymbol{y}_{i,j}^k. \tag{3.45}$$

$$\boldsymbol{\mathcal{B}} \boldsymbol{u}_{i,j}^k + \boldsymbol{V}_{,j}^k \boldsymbol{u}_i^k + \boldsymbol{V}^k \boldsymbol{u}_{i,j}^k = \Lambda_{i,j}^k \boldsymbol{u}_i^k + \Lambda_i^k \boldsymbol{u}_{i,j}^k. \tag{3.46}$$

After multiplying both sides of (3.45) and (3.46) with $(\boldsymbol{y}_i^k)^{\mathrm{T}}$ and $(\boldsymbol{u}_i^k)^{\mathrm{T}}$ respectively and removing the iteration index for simplicity, by keeping in mind this should be done in each iteration, we get

$$-\boldsymbol{y}_i^{\mathrm{T}} \boldsymbol{D}_{2n}^{(2)} \boldsymbol{y}_{i,j} + \boldsymbol{y}_i^{\mathrm{T}} \boldsymbol{Q}_{,j} \boldsymbol{y}_i + \boldsymbol{y}_i^{\mathrm{T}} \boldsymbol{Q} \boldsymbol{y}_{i,j} = \boldsymbol{y}_i^{\mathrm{T}} \Lambda_{i,j} \boldsymbol{y}_i + \boldsymbol{y}_i^{\mathrm{T}} \Lambda_i \boldsymbol{y}_{i,j},$$

$$-\boldsymbol{u}_i^{\mathrm{T}} \boldsymbol{\mathcal{B}} \boldsymbol{u}_{i,j} + \boldsymbol{u}_i^{\mathrm{T}} \boldsymbol{V}_{,j} \boldsymbol{u}_i + \boldsymbol{u}_i^{\mathrm{T}} \boldsymbol{V} \boldsymbol{u}_{i,j} = \boldsymbol{u}_i^{\mathrm{T}} \Lambda_{i,j} \boldsymbol{u}_i + \boldsymbol{u}_i^{\mathrm{T}} \Lambda_i \boldsymbol{u}_{i,j},$$

and with a simple arrangement it is easy to handle

$$[-\boldsymbol{y}_i^{\mathrm{T}} \boldsymbol{D}_{2n}^{(2)} + \boldsymbol{y}_i^{\mathrm{T}} \boldsymbol{Q}\,] \boldsymbol{y}_{i,j} + \boldsymbol{y}_i^{\mathrm{T}} \boldsymbol{Q}_{,j} \boldsymbol{y}_i = \boldsymbol{y}_i^{\mathrm{T}} \Lambda_{i,j} \boldsymbol{y}_i + \boldsymbol{y}_i^{\mathrm{T}} \Lambda_i \boldsymbol{y}_{i,j}, \tag{3.47}$$

and

$$[-\boldsymbol{u}_i^{\mathrm{T}} \boldsymbol{\mathcal{B}} + \boldsymbol{u}_i^{\mathrm{T}} \boldsymbol{V}\,] \boldsymbol{u}_{i,j} + \boldsymbol{u}_i^{\mathrm{T}} \boldsymbol{V}_{,j} \boldsymbol{u}_i = \boldsymbol{u}_i^{\mathrm{T}} \Lambda_{i,j} \boldsymbol{u}_i + \boldsymbol{u}_i^{\mathrm{T}} \Lambda_i \boldsymbol{u}_{i,j}, \tag{3.48}$$

where $\boldsymbol{y}_i$ ($\boldsymbol{u}_i$) and $\boldsymbol{y}_{i,j}$ ($\boldsymbol{u}_{i,j}$) are the eigenvectors and partial derivative of the eigenvectors with respect to q_j (V_j) corresponding to the ith eigenvalue. The expression in brackets in the last two equations are equal to $\Lambda_i \boldsymbol{y}_i^{\mathrm{T}}$ and $\Lambda_i \boldsymbol{u}_i^{\mathrm{T}}$ which can be easily seen from (3.41) and (3.42) by using the symmetry property of the matrices $\boldsymbol{D}_{2n}^{(2)}$, $\boldsymbol{Q}$, $\boldsymbol{\mathcal{B}}$ and $\boldsymbol{V}$. Therefore, after canceling the common terms in both sides of (3.47) and (3.48) and using the orthonormality of eigenvectors $\boldsymbol{y}_i$ and $\boldsymbol{u}_i$ respectively the last two equations take the forms

$$\Lambda_{i,j} = \boldsymbol{y}_i^{\mathrm{T}} \boldsymbol{Q}_{,j} \boldsymbol{y}_i. \tag{3.49}$$

$$\Lambda_{i,j} = \boldsymbol{u}_i^{\mathrm{T}} \boldsymbol{V}_{,j}\, \boldsymbol{u}_i. \tag{3.50}$$

Due to the structure of $\boldsymbol{Q}$ and $\boldsymbol{V}$ the matrices $\boldsymbol{Q}_{,j}$ and $\boldsymbol{V}_{,j}$ have only non-zero elements in their jth and $(2n+1-j)$th diagonal elements, both are 1. As a consequence, we will calculate the Jacobian matrices $\boldsymbol{T}'(q^k)$ by formulas (3.49) and (3.50) depending on the methods used . Again, it is important that it should be calculated in every iteration step in contrast to methods for regular inverse S-L problem, see e.g. [3, 4].

3.2.2 Regularization Method

We use a regularization technique similar to [41] and [67], i.e., a Newton-type method. Let us first come back to the equation (3.43). This equation can not be solved directly because of the condition number of the Jacobian matrix, which gives a measure for the amplification of input inaccuracies. The condition number is defined by $\|(\boldsymbol{T}'(q^k)^{-1}\| \, \|\boldsymbol{T}'(q^k\|$ indeed if $\|.\|$ is L_2 norm it is the ratio of the largest singular value of the $\boldsymbol{T}'(q^k)$ to the smallest, increases rapidly after each iteration since we are faced with an ill-conditioned problem, see Table 3.1.

Table 3.1: Singular values of the Jacobian matrix after each iteration step for harmonic oscillator example in the case $l = 7$, $n = 14$

1. iteration	2. iteration	3. iteration	4. iteration	5. iteration
1.0400531126	1.0559558703	1.1145072672	1.1537342403	1.1735723266
0.5293050705	0.6675954852	0.6382652591	0.6202549015	0.6186132532
0.3971032489	0.5203676842	0.5127079149	0.4946877470	0.4808887875
0.3303938746	0.4176492184	0.4346768956	0.4170291280	0.4023958696
0.2890037709	0.3477198671	0.3774026582	0.3565325589	0.3591043224
0.2603938750	0.3012699019	0.3341463623	0.3278916915	0.3335624512
0.2405064562	0.2755289646	0.3171847648	0.3134653829	0.3182804953
0.2382920547	0.2570813572	0.3031528170	0.3071959075	0.3093702109
0.2233203934	0.2368017918	0.2870271114	0.2983890544	0.2906639244
0.2110322617	0.2311475209	0.2560321132	0.2610719342	0.2779183562
0.1990325255	0.1949670183	0.2138389181	0.1473479378	0.0743480166
0.1894821804	0.1829324255	0.0484895699	0.0043794366	0.0004493142
0.0765460162	0.0292405280	0.0033857039	0.0000212571	0.0000001546
0.0062072726	0.0046273881	0.0000153561	0.0000003699	0.0000000002

To obtain a good approximation for $\Delta\boldsymbol{q}^k$ we need a regularization technique for the linear system (3.43) in each iteration step. This means, we have to approximate the ill-conditioned equation by a suitable well-conditioned equation system, i.e., we have to stabilized the solution process in determining Newton's update. For the solution

of Newton's update according to (3.43), a general representation for regularization methods gives

$$\Delta \boldsymbol{q}^k = \Delta \boldsymbol{q}^k_\gamma = g_\gamma \left((\boldsymbol{A}^k)^{\mathrm{T}} \boldsymbol{A}^k \right) (\boldsymbol{A}^k)^{\mathrm{T}} \boldsymbol{T}(q^k) \tag{3.51}$$

in which $\boldsymbol{A}^k := \boldsymbol{T}'(q^k)$ defined by (3.49),

$$g_\gamma : [0, \theta] \to \mathbb{R}, \quad \theta = \|\boldsymbol{A}^k\|^2$$

is a piecewise defined continuous filter function and the parameter $\gamma > 0$ is called the regularization parameter, see [23] and [45]. Roughly spoken, the included filter is able to make the equation system well-conditioned. The choice $g_\gamma(\sigma_i^2) = \frac{1}{\sigma_i^2 + \gamma}$ leads to the historical Tikhonov-Phillips regularization

$$g_\gamma((\boldsymbol{A}^k)^{\mathrm{T}} \boldsymbol{A}^k) = ((\boldsymbol{A}^k)^{\mathrm{T}} \boldsymbol{A}^k + \gamma I)^{-1}.$$

In other words, to derive regularized solution represented by singular values of Jacobian matrix suppose that $\Delta \boldsymbol{q}^k$ is in the orthogonal complement of the null space of $\boldsymbol{A}^k$ and let $(\sigma_i; \boldsymbol{u}_i, \boldsymbol{v}_i)$ be the singular system of $\boldsymbol{A}^k$, then

$$\Delta \boldsymbol{q}^k = \sum_{i=1}^{n} \left\langle \Delta \boldsymbol{q}^k, \boldsymbol{u}_i \right\rangle \boldsymbol{u}_i$$

and by using the property $(\boldsymbol{A}^k)^{\mathrm{T}} \boldsymbol{A}^k \boldsymbol{u}_i = \sigma_i^2 \boldsymbol{u}_i$ we get

$$[(\boldsymbol{A}^k)^{\mathrm{T}} \boldsymbol{A}^k + \gamma I] \Delta \boldsymbol{q}^k = \sum_{i=1}^{n} (\sigma_i^2 + \gamma) \left\langle \Delta \boldsymbol{q}^k, \boldsymbol{u}_i \right\rangle \boldsymbol{u}_i.$$

After this we derive the regularized solution $\Delta \boldsymbol{q}^k_\gamma$ as

$$\begin{aligned}
\Delta \boldsymbol{q}^k_\gamma &= [(\boldsymbol{A}^k)^{\mathrm{T}} \boldsymbol{A}^k + \gamma \boldsymbol{I}]^{-1} (\boldsymbol{A}^k)^{\mathrm{T}} \boldsymbol{T}(q^k) = \sum_{i=1}^{n} \frac{1}{\sigma_i^2 + \gamma} \left\langle (\boldsymbol{A}^k)^{\mathrm{T}} \boldsymbol{T}(q^k), \boldsymbol{u}_i \right\rangle \boldsymbol{u}_i \\
&= \sum_{i=1}^{n} \frac{1}{\sigma_i^2 + \gamma} \left\langle \boldsymbol{T}(q^k), \boldsymbol{A}^k \boldsymbol{u}_i \right\rangle \boldsymbol{u}_i = \sum_{i=1}^{n} \frac{\sigma_i}{\sigma_i^2 + \gamma} \left\langle \boldsymbol{T}(q^k), \boldsymbol{v}_i \right\rangle \boldsymbol{u}_i \\
&= \sum_{i=1}^{n} g_\gamma(\sigma_i^2) \sigma_i \left\langle \boldsymbol{T}(q^k), \boldsymbol{v}_i \right\rangle \boldsymbol{u}_i.
\end{aligned}$$

In addition, it is possible to take $\boldsymbol{D}^{\boldsymbol{T}} \boldsymbol{D}$ instead of the identity matrix $\boldsymbol{I}$, e.g., with any suitable differentiation matrix $\boldsymbol{D}$. This method is called generalized Tikhonov-Phillips (TP) regularization which is more suitable for our problem. This kind of choice penalizes non-smooth "solutions". Here the second order Hermite differentiation matrix, see [27], is considered as a penalizing matrix.

Now we are able to write the Newton's update as a regularized solution of (3.43) by using the generalized TP regularization scheme

$$\Delta \boldsymbol{q}^k = \Delta \boldsymbol{q}^k_\gamma = [(\boldsymbol{T}'(q^k))^{\mathrm{T}} \boldsymbol{T}'(q^k) + \gamma (\boldsymbol{D}^{(2)})^{\mathrm{T}} \boldsymbol{D}^{(2)}]^{-1} (\boldsymbol{T}'(q^k))^{\mathrm{T}} \boldsymbol{T}(q^k) \tag{3.52}$$

in which the regularization parameter γ should be chosen in a suitable way. We use L-Curve and generalized cross validation (GCV) methods for this purpose. For the first one one can plots the logarithm of the norm of the regularized solution multiplied by penalizing matrix $\boldsymbol{D}$, i.e., $\|\boldsymbol{D}\, \Delta \boldsymbol{q}^k_\gamma\|_2$, against the norm of the regularized residual, i.e., $\|\boldsymbol{T}'(q^k)\Delta \boldsymbol{q}^k_\gamma - \boldsymbol{T}(q^k)\|_2$, for various values of the regularization parameter γ. Since this curve generally has an L-shaped picture it has a corner point which gives us the regularization parameter in each iteration. It is possible to use the curvature of the curve whose maximum identify the corner. For the second one the functional defined in (2.31) has a minimum at desired regularization parameter. More details for these methods was given in the previous chapter.

Furthermore, regarding the nonlinear system (3.37) and (3.38) we need to control the number of iteration step among other things with respect to the "noisy" data $(\lambda_i^{\mathrm{sing}})^\delta$.The number of iteration steps can also act as a regularization parameter $\tilde{\gamma}$, i.e., $\tilde{\gamma} = 1/k$. The total error in solving the problem consist of two parts, namely, the data error term and the approximation error term. Whereas generally the data error term increases during the iteration process the approximation error term decreases. Therefore, the total error has a minimum after certain iteration steps, i.e., one has to stop the iteration process (outer regularization) suitably. Otherwise the total error would start to increase after decreasing during the first iteration steps (Figure 3.1).

To terminate the Newton iteration we use a kind of discrepancy principle, i.e., choose a $\tau > 0$ and accept the iterate q_N as an approximation to solution for which

$$\|(\lambda^{\mathrm{sing}})^\delta - \Lambda(q_N)\|_2 \leq \tau\delta < \|(\lambda^{\mathrm{sing}})^\delta - \Lambda(q_k)\|_2, \quad k = 1, \ldots, N-1.$$

Concerning the convergence properties (for noiseless data) of such a Newton method, we remark that under certain conditions on $\boldsymbol{T}$, $\boldsymbol{T}'$ and $\boldsymbol{B}^\sharp$, see [55], the Newton method in using an outer inverse $\boldsymbol{B}^\sharp$ (i.e., $\boldsymbol{B}^\sharp \boldsymbol{B} \boldsymbol{B}^\sharp = \boldsymbol{B}^\sharp$)

$$\boldsymbol{q}^{k+1} = \boldsymbol{q}^k - \boldsymbol{B}(q^k)^\sharp \boldsymbol{T}(q^k),$$

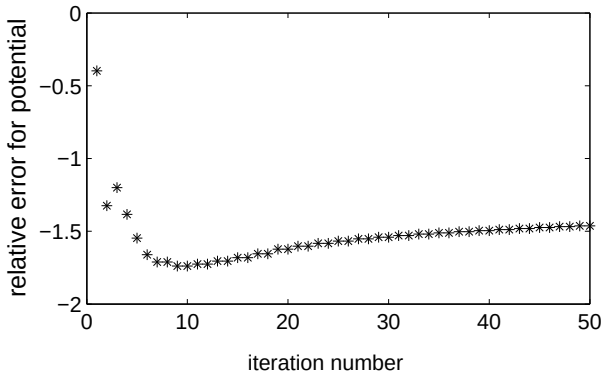

Figure 3.1: Behaviour of the relative error for potential ($\frac{\|q^k - q^{\text{ex.}}\|_2}{\|q^{\text{ex.}}\|_2}$) as a function of iteration number in a semilog picture. It can be seen that error is increasing after 10. iteration. In this computation we use noisy data with %19 noise for harmonic oscillator, $l = 9$, $n = 26$.

where $\boldsymbol{B}(q^k)$ is an approximation of the Jacobian $\boldsymbol{T}'(q^k)$, is still linearly convergent even for a singular Jacobian. Our Jacobians, see Table 3.1, are "almost or nearly" singular. If one uses the outer inverse $\boldsymbol{T}'(q^k)^\sharp$ instead of an approximation $\boldsymbol{B}(q^k)^\sharp$ Newton's method even converges quadratically. TP regularization provides not an outer inverse of the Jacobian but only an approximate outer inverse which, fortunately, serves as an approximate regularizer, see [54]. This is in good agreement with our observations on the numerical results in the next chapter.

CHAPTER 4

ALGORITHM AND NUMERICAL RESULTS

In this chapter we describe an algorithm corresponding to detailed information of the previous chapters and illustrate the numerical results with examples both.

4.1 Algorithm for Non-Polynomial Case

INPUT : n-number of eigenvalues, eigenvalue set $\left\{\lambda_j\right\}_{j=1}^{n}$, tolerance number ϵ ($\tau\delta$ in noisy case if noise level δ is known), maximum iteration number $N_{\max}$, and truncation parameter l for infinite interval.

◦ Set $h = \frac{2l}{2n+1}$ and determine grid points as $x = [x_1 = -l + h : h : x_{2n} = l - h]$ (Note that we have $2n$ grid points),

◦ Choose the initial potential $\boldsymbol{q}^k$ as a function calculated at half grid points, i.e., $\left\{x_j\right\}_{j=1}^{n}$.

▹ *while eigenvalue residual* $> \epsilon$ or *eigenvalue residual* $> \tau\delta$ (for noisy data with noise level δ) or $k < N_{\max}$

◦ $\tilde{q}^k = [q^k(x_1), \ldots, q^k(x_n), q^k(x_n), \ldots, q^k(x_1)]$ which is full initial potential,

◦ Calculate eigenvalues Λ and eigenvector for $\tilde{\boldsymbol{q}}^k$ via pseudospectral method by using (3.37). It should be mentioned that since the accuracy of the pseudospectral method is more better if it uses bigger dimensional matrices we calculate first $2n$ eigenvalues and eigenvectors to obtain first n eigenvalues more accurately. So according to (3.37) we have $(2n * 2n)$ system which is

$$(-\boldsymbol{D}^{(2)}_{2n*2n} + \boldsymbol{Q}_{2n*2n})y = \Lambda \boldsymbol{y}, \quad \boldsymbol{Q} = \mathrm{diag}(\tilde{\boldsymbol{q}}^k),$$

◦ Construct Jacobian matrix by using formula (3.49),

◦ Construct right hand side of (3.43) which is $\boldsymbol{T}(\boldsymbol{q}^k) = \lambda_i^{\text{sing}} - \Lambda_i^k$, $i = 1, \ldots, n$,

◦ Calculate $\Delta\boldsymbol{q}^k$ by using generalized Tikhonov-Phillips Regularization scheme in (3.52),

◦ Update potential by (3.44)

◦ Calculate $resid = \|\boldsymbol{T}(q^k)\|_2$,

◦ $\boldsymbol{q}^k \leftarrow \boldsymbol{q}^{k+1}$, $k = k + 1$

▹ *end*

OUTPUT : $q = [q^k(x_3), \ldots, q^k(x_n), q^k(x_n), \ldots, q^k(x_3)]$, here we omit the first two (respectively last two) value of the computed potential. According to our numerical experiments in test problems, we get poor results at first two grid points without giving "excellent" initial potential.

4.1.1 Numerical Examples

We apply our algorithms to reconstruct two symmetric potentials which are quantum mechanical harmonic oscillator, i.e., $q(x) = x^2$ and symmetric double well potential (SDWP), i.e., $q(x) = ax^4 + bx^2 + c$ with $a = 0.6$, $b = -8$, $c = 40$ and $x \in (-\infty, \infty)$ for both cases.

Quantum Mechanical Harmonic Oscillator Potential

The first example, which is very well known, has analytic solution and the exact eigenvalue set $\lambda_i^{\text{sing}} = 2i + 1$, $i = 1, \ldots$ for the direct problem. We use the exact eigenvalues in our algorithm for this example. For a given finite set of eigenvalues, we present the reconstructed potential and illustrate some convergence properties according to different truncation values L, namely $l = 7$, $l = 8$, and $l = 9$. All computational efforts were done with the same maximum iteration number, $N_{\max} = 50$ and we give termination criteria ϵ depending on examples for Newton-like method. But

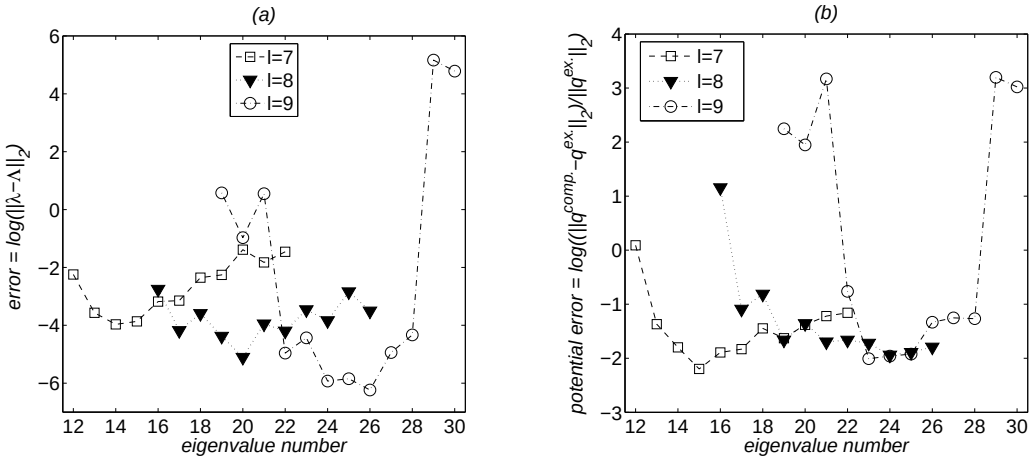

Figure 4.1: Behavior of the (a) residual error $\|\Lambda - \lambda^{\text{sing}}\|$, (b) relative potential error $\frac{\|q^k - q^{\text{ex.}})\|_2}{\|q^{\text{ex.}}\|_2}$ as a function of used eigenvalue number for Harmonic oscillator with different L values. Initial potentials are $0.4 * q^{\text{ex.}}$, $0.5 * q^{\text{ex.}}$ and $0.6 * q^{\text{ex.}}$ respectively.

initial potential and number of used eigenvalues differ depending on the truncation parameter.

In Figure 4.1, we present the graph of the error for residual and potential according to number of used eigenvalues for different truncation parameters. We observe that both errors have nearly same behaviour. Therefore we can use the residual error to determine which number of used eigenvalue is the best one for each truncation parameter. When l is small we observe that computed potentials converge to exact potential for all number of eigenvalues we used. On the other hand for bigger truncation number the range of used eigenvalue numbers for convergence is more smaller, such as constructed potential does not converge to exact potential for $n = 20, 21, 29, 30$ in the $l = 9$ case. By means of these behaviours we can conclude that we need more eigenvalues to get convergence to the exact potential when l increases in the limiting case.Also it should be noted that initial potential has a vital role in this picture, i.e., worse choices of initial potential causes a restriction on the number of used eigenvalues.

We look at the convergence rate of the method under the suitable choices of initial potential and number of used eigenvalues, see Figure 4.2. Under these assumptions we observe that the convergence rate is linear as we expected because of the approximated Jacobian in the Newton-like method. In addition, the similar behaviour should

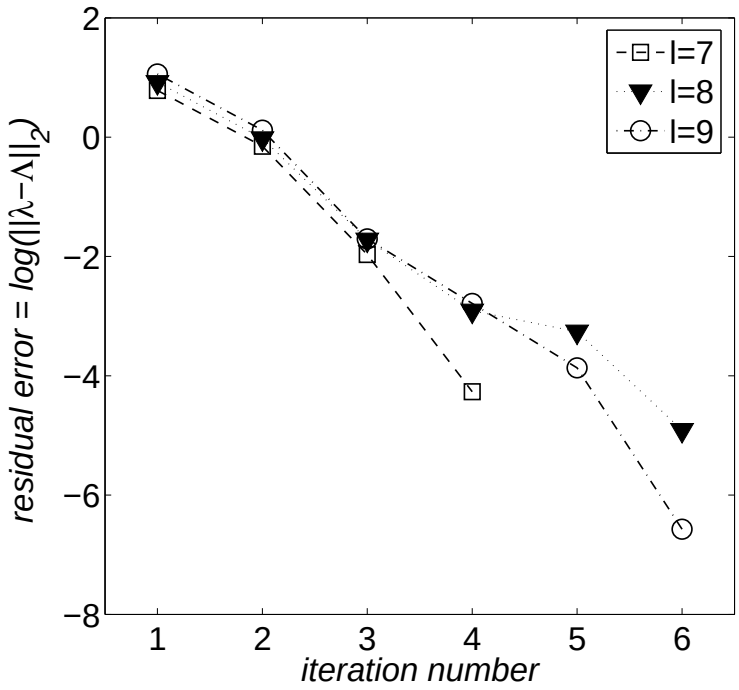

Figure 4.2: The logarithm of the $\Lambda - \lambda^{\text{sing}}$ versus iteration number. Here q^0 is same for all three cases, and number of used eigenvalues are 14,19,26 for $l = 7, 8, 9$ respectively.

be seen for L_2 and L_∞ errors (relative) for potential from the Table 4.1. And Figure 4.3 represents the reconstructed potential for the considered truncation parameters with exact solution and the spline which uses the computed values at grid points. Moreover we used the Levenberg-Marquardt method as a regularization method with L-Curve parameter choice rule. Iteratively regularized Gauss-Newton method does not give convergent results. This may cause from the initial potential. On the other hand Generalized cross validation gives the similar results with L-curve method.

Symmetric Double Well Potential (SDWP)

As a second example we took SDWP $q(x) = 0.6x^4 - 8bx^2 + 40$ which has spectrum containing four nearly degenerate eigenvalues, namely the first eight eigenvalues. Because of this eigenvalue pattern recovery of SDWP type potentials needs more sensitive conditions on used eigenvalue numbers and initial potential than previous example. Additionally we can not increase truncation parameter as fast as before and

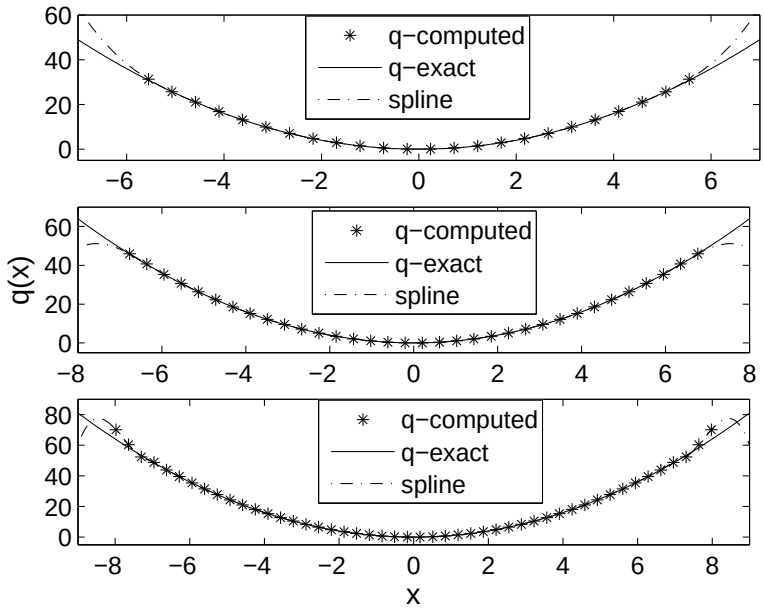

Figure 4.3: Reconstructed potential at grid points for $l = 7, 8, 9$ with corresponding number of used eigenvalues 14, 19, 26 respectively.

it should not so big. In this example it does not make sense to take $l > 5.5$ taking into account the number of used eigenvalues and necessity of good initial potential. This implies that without giving high eigenvalue number and good initial guess we have no convergence for computed potential. It can be seen in Figure 4.4 that even in $l = 5.5$ case we need more than 30 eigenvalues and this value reaches more than 45 for $l = 6$. Unfortunately it is not easy to supply too many eigenvalues accurately in experimental point of view. On the other hand initial potential must be close to exact potential for bigger l. For example we take $q^0 = 0.7 * q^{\text{ex.}}$ for $l = 6$ to obtain

Table 4.1: L_2 and L_∞ errors(relative) of potential after each iteration for Harmonic oscillator in the case $l = 8$ and $N = 19$ with $q^0 = 0.4 * q^{ex.}$

k	$\frac{\|q^k - q^{\text{ex.}}\|_2}{\|q^{\text{ex.}}\|_2}$	$\frac{\|q^k - q^{\text{ex.}})\|_\infty}{\|q^{ex.}\|_\infty}$
1	0.132117	0.258226
2	0.036065	0.070489
3	0.021378	0.041784
4	0.017385	0.033979
5	0.016970	0.033169
6	0.016869	0.032972

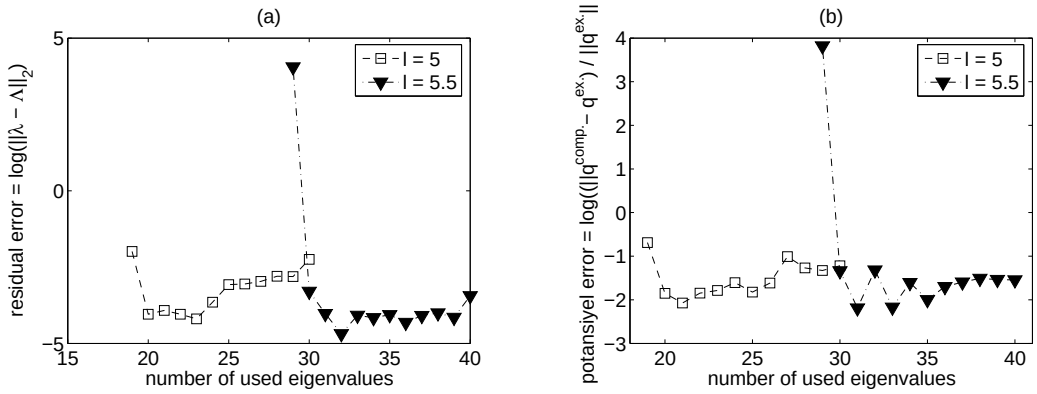

Figure 4.4: Behavior of the (a) residual error $\|\Lambda - \lambda^{\text{sing}}\|$, (b) relative potential error $\frac{\|q^k - q^{\text{ex.}})\|_2}{\|q^{\text{ex.}}\|_2}$ as a function of used eigenvalue number for SDWP with different l values.

convergence to exact potential while we use less sensitive ones for $l = 5$ and $l = 5.5$. In the SDWP example we get the same convergence rate which is linear as before

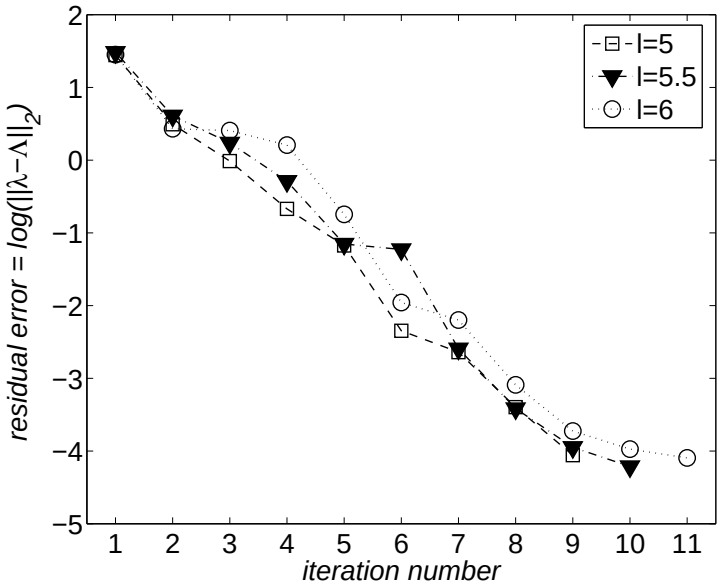

Figure 4.5: The logarithm of the $\Lambda - \lambda^{\text{sing}}$ versus iteration number for SDWP. Here q^0 are $0.4 * q^{\text{ex.}}$, $0.5 * q^{\text{ex.}}$, $0.7 * q^{\text{ex.}}$ and number of used eigenvalues are 23,31,48 for $l = 5, 5.5, 6$ respectively.

under mentioned condition (Figure 4.5). And Figure 4.6 presents the reconstructed SDWP potentials for $l = 5$ (upper), 5.5, 6 (lower).

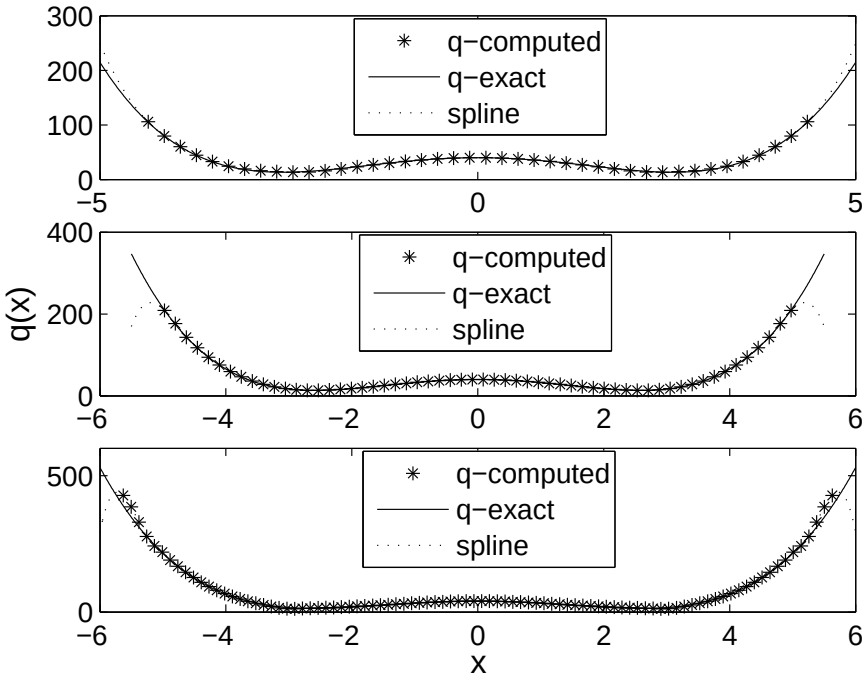

Figure 4.6: Computed potentials for SDWP with $l = 5, 5.5, 6$ and corresponding number of used eigenvalues 23, 31, 48 respectively.

4.2 Algorithm for Polynomial (Hermite Polynomials) Case

INPUT : n-number of eigenvalues, eigenvalue set $\left\{\lambda_j\right\}_{j=1}^{n}$, tolerance number ϵ, maximum iteration number $N_{\max}$, scaling parameter α.

∘ Determine the nodes ξ as a roots of the Hermite polynomials of order $2n$ and calculate scaling nodes as $x = \frac{\xi}{\alpha}$.

∘ Choose the initial potential $\boldsymbol{q}^k$ as a function calculated at scaled half grid points, i.e., $\left\{x_j\right\}_{j=1}^{n}$.

▹ *while eigenvalue residual* $> \epsilon$ or $k < N_{\max}$

∘ $\tilde{q}^k = [q^k(x_1), \ldots, q^k(x_n), q^k(x_n), \ldots, q^k(x_1)]$ which is full initial potential,

∘ Calculate eigenvalues Λ and eigenvectors for $\tilde{\boldsymbol{q}}^k$ via Hermite pseudospectral method in which modified potential $V(x)$ given in (3.24) is used. It should be mentioned that since the accuracy of the pseudospectral method is more better if it uses

bigger dimensional matrices we calculate first $2n$ eigenvalues and eigenvectors to obtain first n eigenvalues and eigenvectors more accurately. So according to (3.37) we have $(2n * 2n)$ system which is

$$(\mathcal{B} + \boldsymbol{V}^k)\boldsymbol{u}^k = \Lambda \boldsymbol{u}^k$$

◦ Construct Jacobian matrix by using formula (3.50),

◦ Construct right hand side of (3.43) which is $T(\boldsymbol{q}^k) = \lambda_i^{\text{sing}} - \Lambda_i^k$, $i = 1, \ldots, n$,

◦ Calculate $\Delta \boldsymbol{V}^k$ by using generalized Tikhonov-Phillips Regularization scheme in (3.52),

◦ Update modified potential by $\boldsymbol{V}^{k+1} = \boldsymbol{V}^k + \Delta \boldsymbol{V}^k$

◦ Calculate $resid = \|\boldsymbol{T}(q^k)\|_2$,

◦ $\boldsymbol{V}^k \leftarrow \boldsymbol{V}^{k+1}$

◦ Evaluate original potential q by the help of (3.24), $k = k + 1$

▹ *end*

OUTPUT : $q = [q^k(x_1), \ldots, q^k(x_n), q^k(x_n), \ldots, q^k(x_1)]$, k

4.2.1 Numerical Examples

In this section we give two different potential examples, namely biswas potential and anharmonic oscillator potential to illustrate the performance of our second algorithm.

Biswas Potential

Our first example, $q(x) = \mu x^2 + \nu x^4$ where μ and ν are parameters, is related with some problems about atomic and molecular properties in quantum chemistry [13]. We take $\mu = \nu = 0.1$ in our experiments. When we try to choose bigger μ and ν such as 1, 10 or more it is not possible to recover the associated potential due to the higher values of $q(x)$. In this case the direct problem does not give accurate results for the complete set

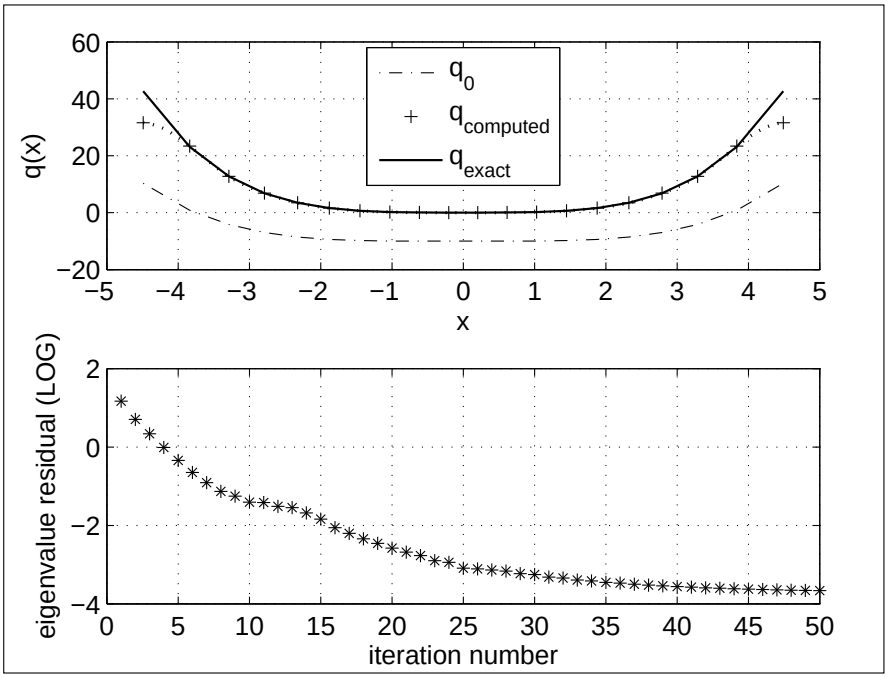

Figure 4.7: Reconstructed potential (upper) and the convergence behaviour of the residual according to iteration number (lower) with 10 eigenvalues using LM and L-curve.

of eigenvalues. Moreover, the determination of the scaling parameter is not an easy duty for high values of parameters. We use the package MATSLISE [48] to supply the eigenvalues which we need to recover potentials in our algorithm. In Figures (4.7)-(4.12) we present the reconstructed potentials with the convergence property of the eigenvalue residual, i.e., $\|\lambda - \Lambda\|_2$. In each figure we use Levenberg-Marquardt (LM) regularization method with L-curve and LM regularization method with Generalized cross validation (GCV). Moreover, the initial potential which is $0.05x^4-10$ is the same for all cases. 10 eigenvalues were used for the reconstruction procedure in Figures 4.7 and 4.8. We try to choose scaling parameter starting from 1 and determine the best one as 1.2 by inspecting the convergence behaviour of the eigenvalue residual. According to convergence graph both methods does not reach the desired accuracy level 10^{-7} with the maximum iteration number 50. Indeed the accuracy does not exceed 10^{-4} because of the inadequate truncation size 20 for the direct computation of the first 10 eigenvalues in the iterative process. In Figures 4.9 and 4.10 20 eigenvalues were used and more satisfactory results were observed. If we compare the iteration number for L-curve and GCV, the second one stops at the 25th iteration while the first

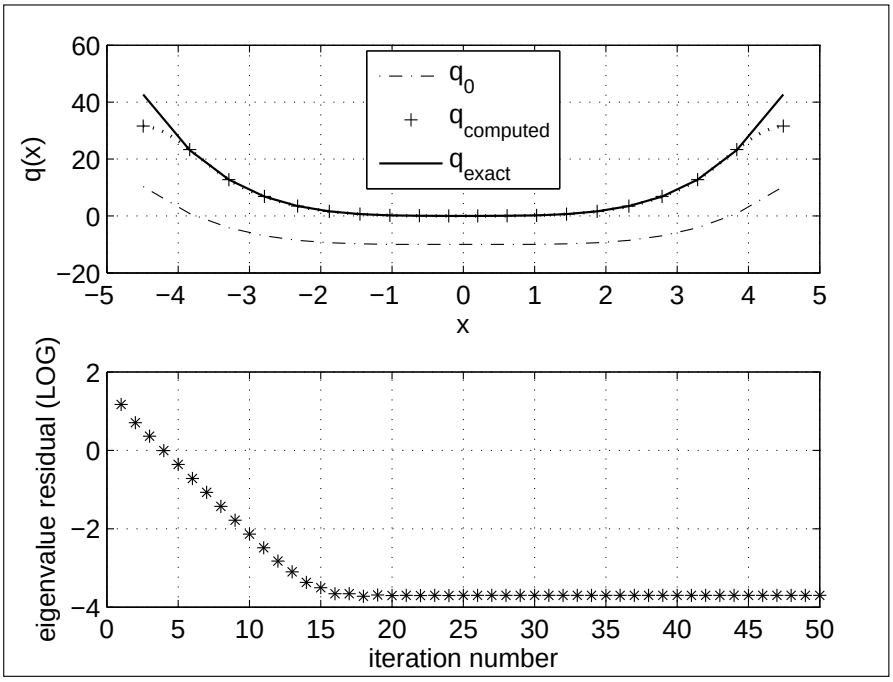

Figure 4.8: Reconstructed potential (upper) and the convergence behaviour of the residual according to iteration number (lower) with 10 eigenvalues using LM and GCV.

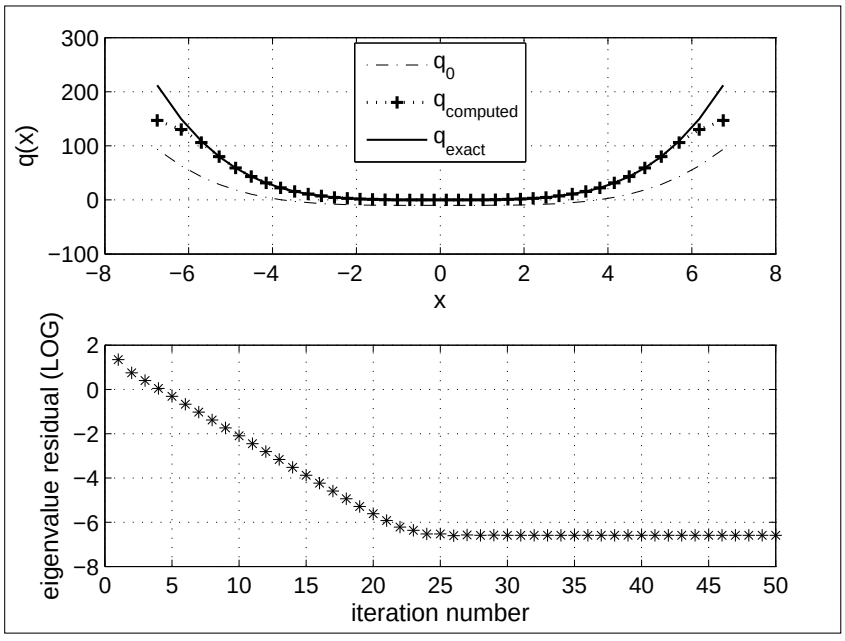

Figure 4.9: Reconstructed potential (upper) and the convergence behaviour of the residual according to iteration number (lower) with 20 eigenvalues using LM and L-curve.

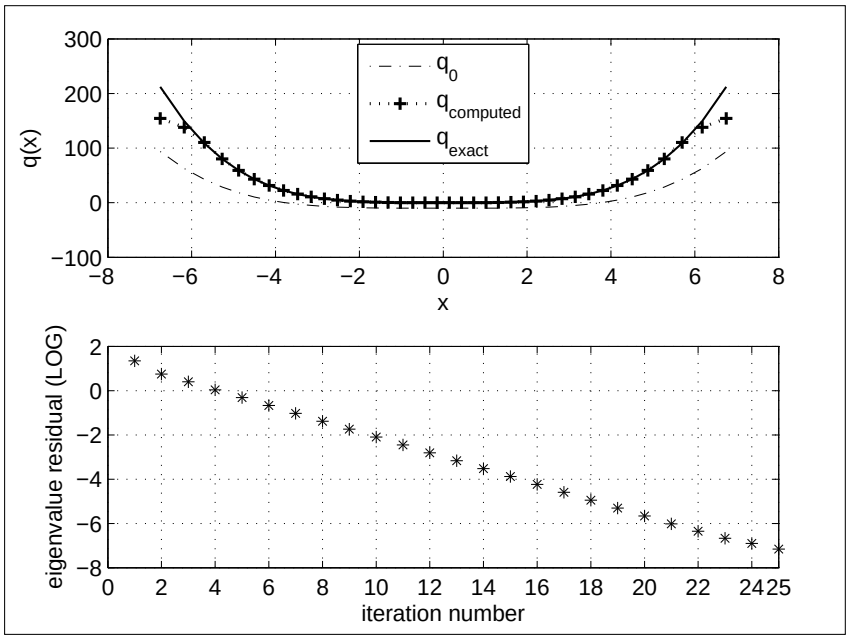

Figure 4.10: Reconstructed potential (upper) and the convergence behaviour of the residual according to iteration number (lower) with 20 eigenvalues using LM and GCV.

one does not reach the desired accuracy with max iteration number. But if we make a little careful inspection on the scaling parameter, L-curve also reaches the desired accuracy with $\alpha = 1.22$ at the 28th iteration. This shows the effect of the scaling parameter on the iteration number. We used 30 eigenvalue to recover the potential in Figures 4.11 and 4.12 with the scaling parameter $\alpha = 1.25$. Both L-curve and GCV with LM work efficiently. Moreover, there is a relation between the scaling parameter and the number of used eigenvalues. Firstly in Figure 4.13 we fixed the scaling parameter α as 1.25 and took different eigenvalue number. We observe from the relative error for potential that the fixed α gives satisfactory convergent results for all used number of eigenvalues, namely 22, 27, 32, 37. But results are not so good, even non convergent in some cases in which eigenvalue number less than 20 or greater than 40. Now, in Figure 4.14 we fixed the used number of eigenvalues as 32 and we look at the behaviours of the relative potential error for different choices of the scaling parameter. It can be seen from this figure there is also rough scaling parameter interval in which we derive very accurate results for a given eigenvalue number. On the other hand results near the boundary are poorer than that of other points. We observe this suffering situation more heavily when we take more eigenvalue number. It seems

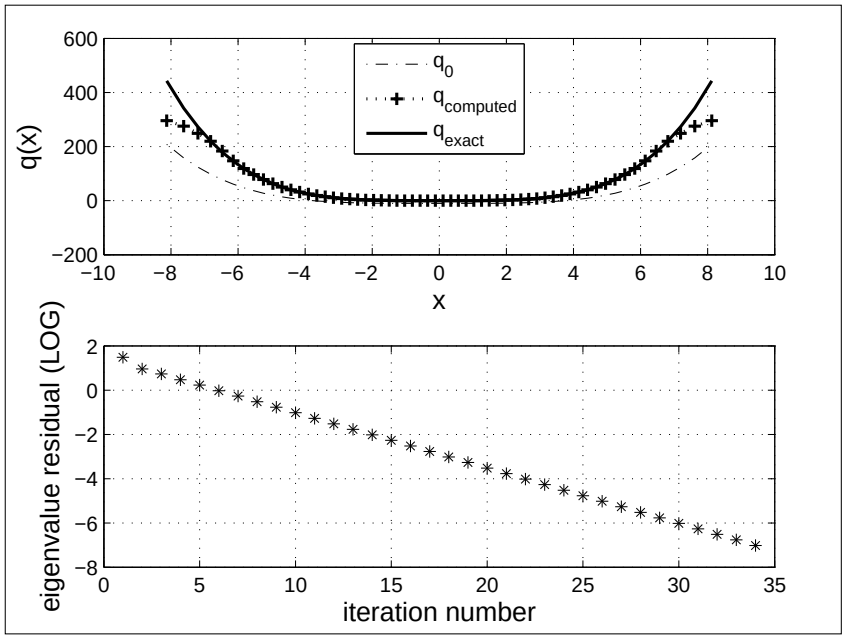

Figure 4.11: Reconstructed potential (upper) and the convergence behaviour of the residual according to iteration number (lower) with 30 eigenvalues using LM and L-curve.

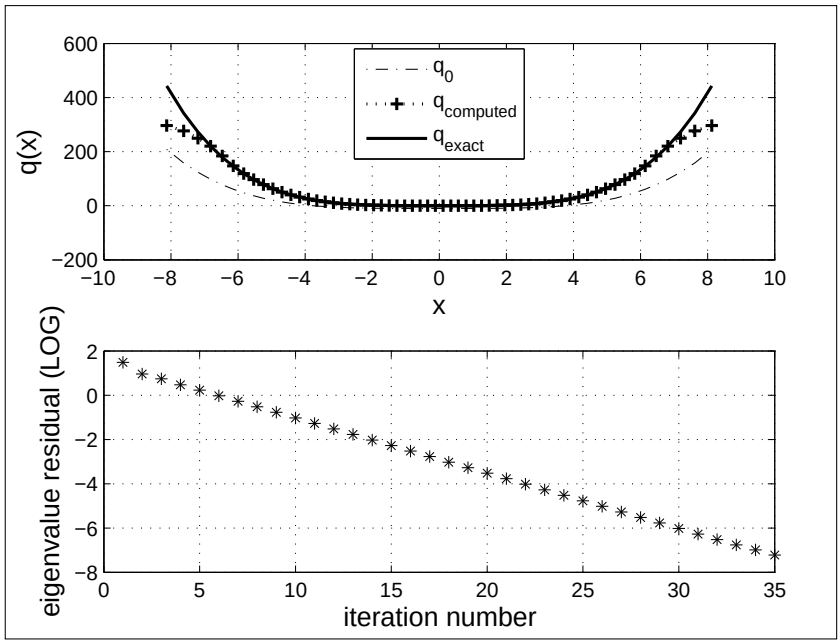

Figure 4.12: Reconstructed potential (upper) and the convergence behaviour of the residual according to iteration number (lower) with 30 eigenvalues using LM and GCV.

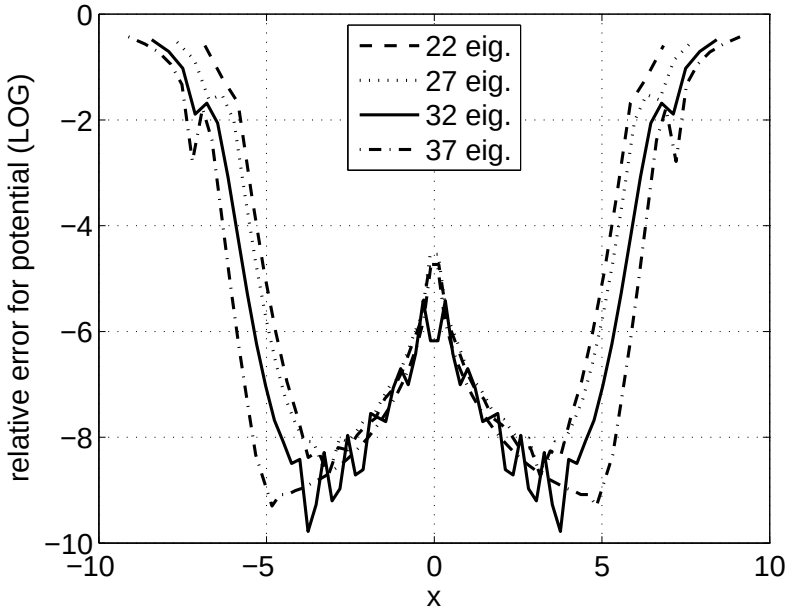

Figure 4.13: Logarithm of the relative error at grid points for fixed scaling parameter α with different eigenvalue number.

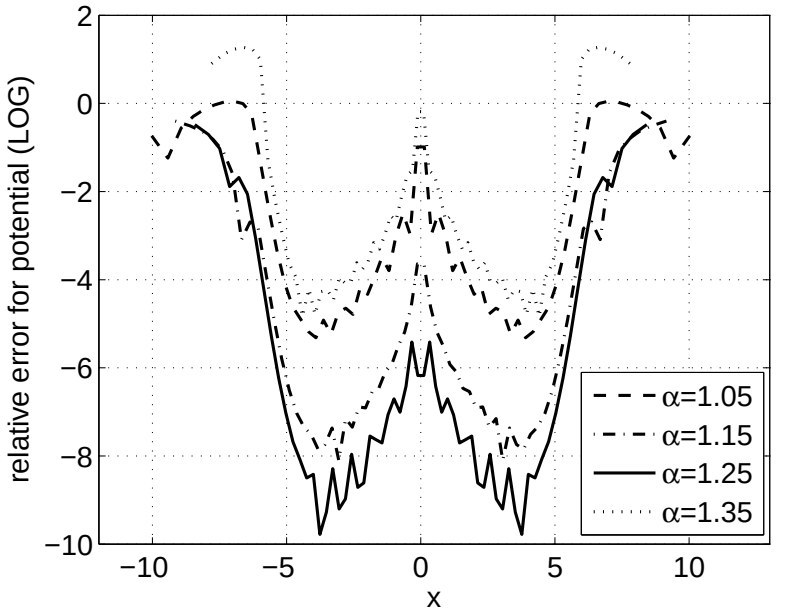

Figure 4.14: Logarithm of the relative error at grid points for fixed eigenvalue number with different scaling parameter α.

that the high value of the potential at the boundary has an effect on this observations. On the other hand, of course, the initial potential has also an effect about these poor results near the boundary. Moreover we report also that iteratively Gauss-Newton method (IRGNM) does not work with neither L-curve nor GCV without giving very good initial potential for this example.

Anharmonic Oscillator Potential

Table 4.2: Relative errors for anharmonic oscillator potential ($a = b = 0.1$) at grid points with different methods.

$a = b = 0.1, \quad \alpha = 1, \quad n = 15$					
j	x_j	LM - L curve $\gamma = 0.0579$	LM - GCV $\gamma = 5.9639$	IRGNM - L curve $\gamma = 9.9825 \times 10^{-8}$	IRGNM - GCV $\gamma = 5.3203 \times 10^{-11}$
1	-6.86	1.32×10^{-1}	8.09×10^{-2}	8.09×10^{-4}	2.01×10^{-3}
2	-6.14	2.35×10^{-2}	1.31×10^{-2}	1.91×10^{-3}	9.16×10^{-4}
3	-5.53	2.60×10^{-3}	1.08×10^{-3}	1.13×10^{-4}	8.18×10^{-5}
4	-4.99	3.89×10^{-4}	1.41×10^{-4}	6.73×10^{-5}	1.09×10^{-5}
5	-4.48	8.71×10^{-5}	2.70×10^{-5}	2.85×10^{-5}	2.15×10^{-6}
6	-4.00	2.90×10^{-5}	7.41×10^{-6}	1.51×10^{-5}	6.00×10^{-7}
7	-3.54	1.42×10^{-5}	2.85×10^{-6}	1.03×10^{-5}	2.34×10^{-7}
8	-3.10	8.93×10^{-6}	1.55×10^{-6}	7.50×10^{-6}	1.30×10^{-7}
9	-2.67	4.90×10^{-6}	1.14×10^{-6}	3.14×10^{-6}	9.83×10^{-8}
10	-2.24	4.86×10^{-7}	9.60×10^{-7}	4.69×10^{-6}	8.75×10^{-8}
11	-1.83	7.05×10^{-6}	6.41×10^{-7}	1.39×10^{-5}	6.26×10^{-8}
12	-1.42	9.80×10^{-6}	2.81×10^{-7}	1.49×10^{-5}	2.39×10^{-8}
13	-1.01	9.89×10^{-7}	2.54×10^{-6}	1.14×10^{-5}	2.50×10^{-7}
14	-0.60	4.32×10^{-5}	7.94×10^{-6}	1.02×10^{-4}	8.05×10^{-7}
15	-0.20	2.29×10^{-4}	3.10×10^{-5}	4.92×10^{-4}	3.18×10^{-6}

We take into account the anharmonic oscillator potential $q(x) = x^2 + \dfrac{ax^2}{1 + bx^2}$ as a second example. Here a and b are positive constants. Anharmonic oscillator has different behaviour depending on the parameters. We take some modified version of x^2 as an initial potential for anharmonic oscillator potential. Actually x^2 gives the best results in each cases.

For the first case, we choose $a = b = 0.1$ in which the potential is similar to harmonic oscillator $q(x) = x^2$. For this potential all methods we proposed in chapter 3 work efficiently. In Table 4.2 we present the relative potential error for all methods with a prescribed parameters a, b, α and n. Number of used eigenvalues effects the scaling parameter and the iteration number in a convergent picture in Figure 4.15. It can be

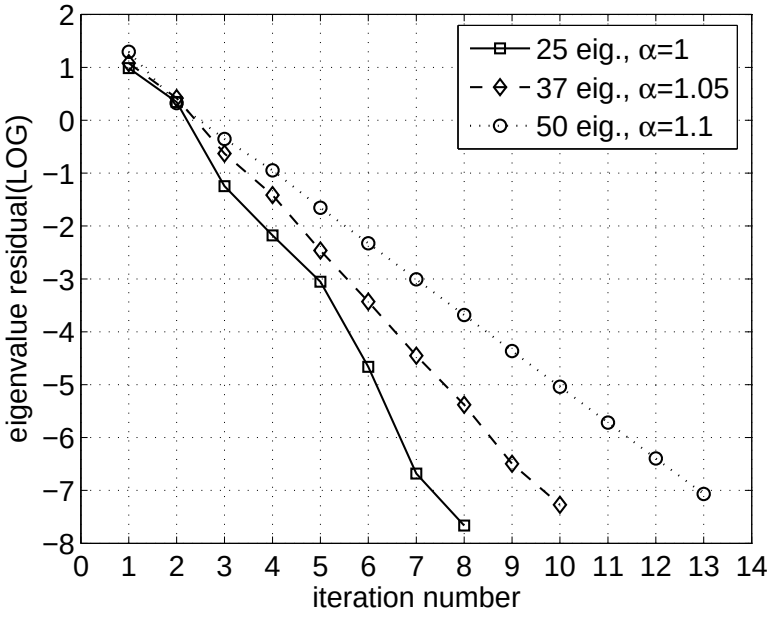

Figure 4.15: Convergence behaviour of the eigenvalue residual with different eigenvalue number and corresponding scaling parameter for anharmonic oscillator ($a = b = 0.1$)

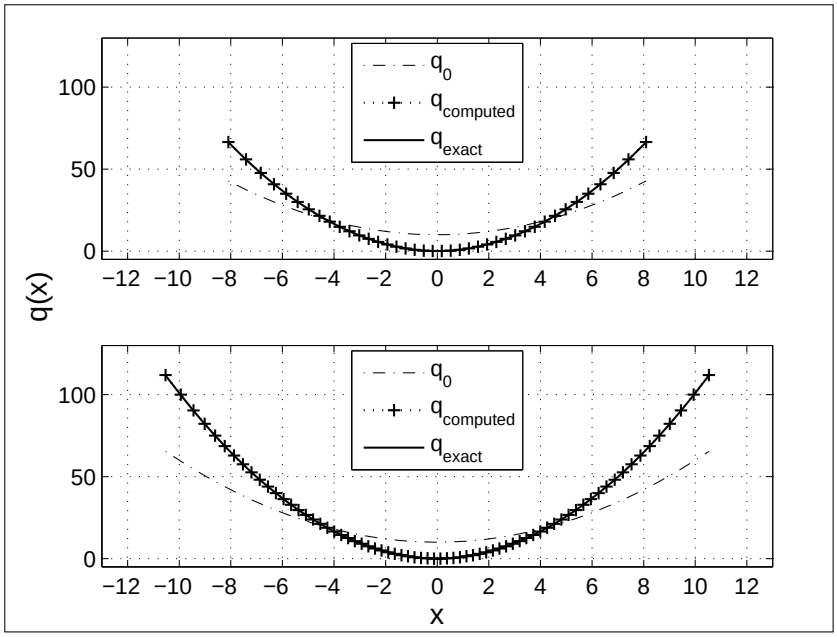

Figure 4.16: Reconstructed potential for anharmonic oscillator ($a = b = 0.1$) with 20 eigenvalues, $\alpha = 1$ (upper) and 35 eigenvalues, $\alpha = 1.05$ (lower)

Table 4.3: Relative errors for anharmonic oscillator potential ($a = b = 1$) at grid points with different methods.

$a = b = 1, \quad \alpha = 1.1, \quad n = 25$					
j	x_j	LM - L CURVE $\gamma = 0.0361$	LM - GCV $\gamma = 1.2437 \times 10^{-6}$	IRGNM - L CURVE $\gamma = 1.8739 \times 10^{-6}$	IRGNM - GCV $\gamma = 2.8722 \times 10^{-12}$
1	-8.35	7.69×10^{-2}	4.71×10^{-2}	2.04×10^{-3}	1.16×10^{-2}
3	-7.25	9.76×10^{-4}	7.19×10^{-3}	4.27×10^{-4}	3.44×10^{-3}
5	-6.39	2.27×10^{-4}	6.42×10^{-4}	5.27×10^{-5}	5.07×10^{-4}
7	-5.64	3.68×10^{-5}	8.37×10^{-5}	3.93×10^{-5}	7.36×10^{-5}
9	-4.94	9.20×10^{-6}	1.81×10^{-5}	2.77×10^{-5}	1.68×10^{-5}
11	-4.28	4.74×10^{-6}	6.52×10^{-6}	2.15×10^{-5}	6.49×10^{-6}
13	-3.65	5.09×10^{-6}	4.00×10^{-6}	8.54×10^{-6}	4.31×10^{-6}
15	-3.04	3.58×10^{-6}	3.60×10^{-6}	6.19×10^{-6}	4.21×10^{-6}
17	-2.44	6.39×10^{-6}	2.66×10^{-6}	1.43×10^{-5}	3.76×10^{-6}
19	-1.86	1.77×10^{-5}	2.99×10^{-6}	9.10×10^{-5}	1.05×10^{-6}
21	-1.28	1.01×10^{-5}	2.02×10^{-5}	1.17×10^{-4}	1.66×10^{-5}
23	-0.71	1.54×10^{-4}	5.99×10^{-5}	6.45×10^{-5}	5.08×10^{-5}
25	-0.14	9.08×10^{-4}	3.24×10^{-4}	1.32×10^{-3}	1.35×10^{-4}

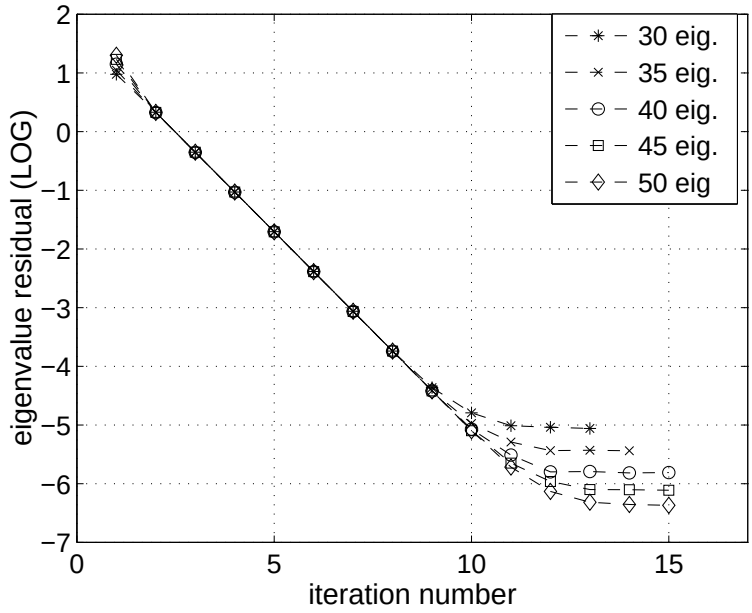

Figure 4.17: Convergence behaviour of the eigenvalue residual with different eigenvalue number and fixed scaling parameter $\alpha = 1.1$ for anharmonic oscillator ($a = b = 1$)

Table 4.4: Relative errors for anharmonic oscillator potential ($a = 10$, $b = 1$) at grid points for different eigenvalue number n.

					$a = 10$, $b = 1$, $\alpha = 1.2$, IRGNM - GCV			
j	x_j	$n = 15$ ($\gamma = 4.1580 \times 10^{-6}$)	x_j	$n = 20$ ($\gamma = 1.2357 \times 10^{-7}$)	x_j	$n = 25$ ($\gamma = 4.2586 \times 10^{-9}$)	x_j	$n = 30$ ($\gamma = 1.2164 \times 10^{-10}$)
1	-5.72	3.65×10^{-2}	-6.75	2.79×10^{-2}	-7.65	2.96×10^{-2}	-8.47	2.34×10^{-2}
3	-4.61	3.87×10^{-4}	-5.70	5.12×10^{-4}	-6.65	1.01×10^{-3}	-7.49	6.17×10^{-4}
5	-3.74	5.11×10^{-4}	-4.88	1.01×10^{-4}	-5.86	2.30×10^{-4}	-6.74	2.04×10^{-4}
7	-2.95	4.65×10^{-4}	-4.15	9.93×10^{-5}	-5.17	5.28×10^{-5}	-6.07	5.97×10^{-5}
9	-2.22	4.89×10^{-4}	-3.47	9.13×10^{-5}	-4.53	1.39×10^{-5}	-5.46	2.13×10^{-5}
11	-1.52	5.66×10^{-4}	-2.83	8.76×10^{-5}	-3.93	3.38×10^{-6}	-4.88	9.34×10^{-6}
13	-0.84	4.73×10^{-4}	-2.21	6.47×10^{-5}	-3.35	1.45×10^{-7}	-4.33	5.05×10^{-6}
15	-0.17	5.03×10^{-3}	-1.61	1.87×10^{-5}	-2.79	8.01×10^{-7}	-3.80	3.40×10^{-6}
17			-1.02	2.47×10^{-4}	-2.24	7.87×10^{-6}	-3.28	2.72×10^{-6}
19			-0.44	6.70×10^{-4}	-1.71	2.64×10^{-5}	-2.78	1.86×10^{-6}
21					-1.18	5.75×10^{-5}	-2.28	7.08×10^{-7}
23					-0.65	1.27×10^{-4}	-1.80	7.05×10^{-6}
25					-0.13	8.09×10^{-4}	-1.31	1.76×10^{-5}
27							-0.83	3.65×10^{-5}
29							-0.36	1.00×10^{-4}

seen from the Figure 4.16 that the bigger scaling parameter is needed for the higher eigenvalue number for the better results. Moreover, the choice of $\alpha = 1.1$ for the scaling parameter also gives satisfactory results almost all n values.

We also test our algorithm with the case $a = b = 1$ in anharmonic oscillator potential. We derive similar observations as in the previous case. Table 4.3 delivers the relative error for the potential for different methods which gives convergent reconstruction. It is possible to obtain more satisfactory results when we increase the eigenvalue number. It can be seen from Figure 4.17 algorithm gives very similar convergence behaviour for the eigenvalue residual with fixed scaling parameter for different eigenvalue number.

In the final case, in which $a = 10$, $b = 1$, the potential has different shape from the cases covered before. We demonstrate the effect of the number of used eigenvalues on a chosen method, namely IRGNM-GCV in the Table 4.4. We obtain satisfactory results in each situation and one reconstructed potential is pictured in Figure 4.18.

On the other hand, we mention about two different Tikhonov-Philips regularization method, namely Tikhonov-Philips and generalized Tikhonov-Philips which give the regularized solutions (2.14) and (2.19) respectively. The difference between them is

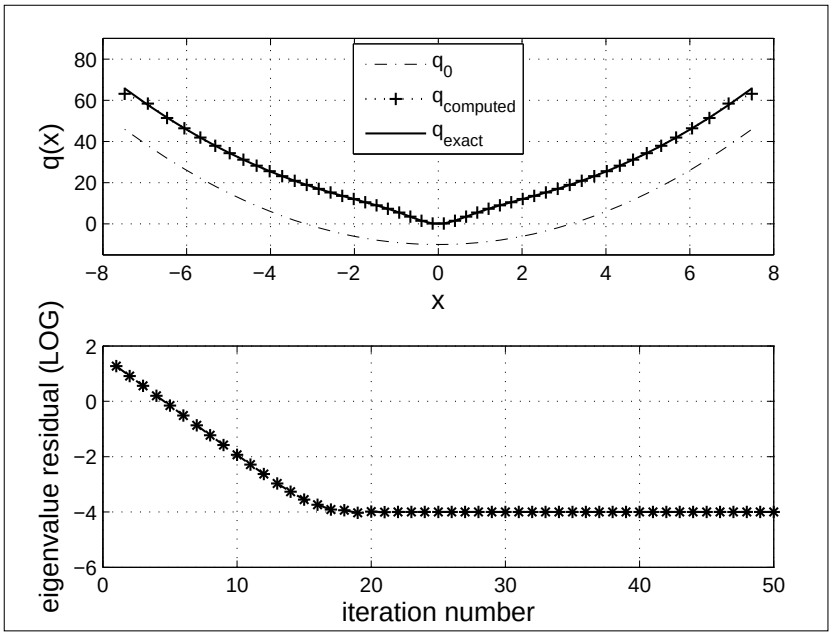

Figure 4.18: Reconstructed potential for anharmonic oscillator ($a = 10$, $b = 1$) with 24 eigenvalues, $\alpha = 1.2$ (upper) and convergence behaviour of the residual (lower).

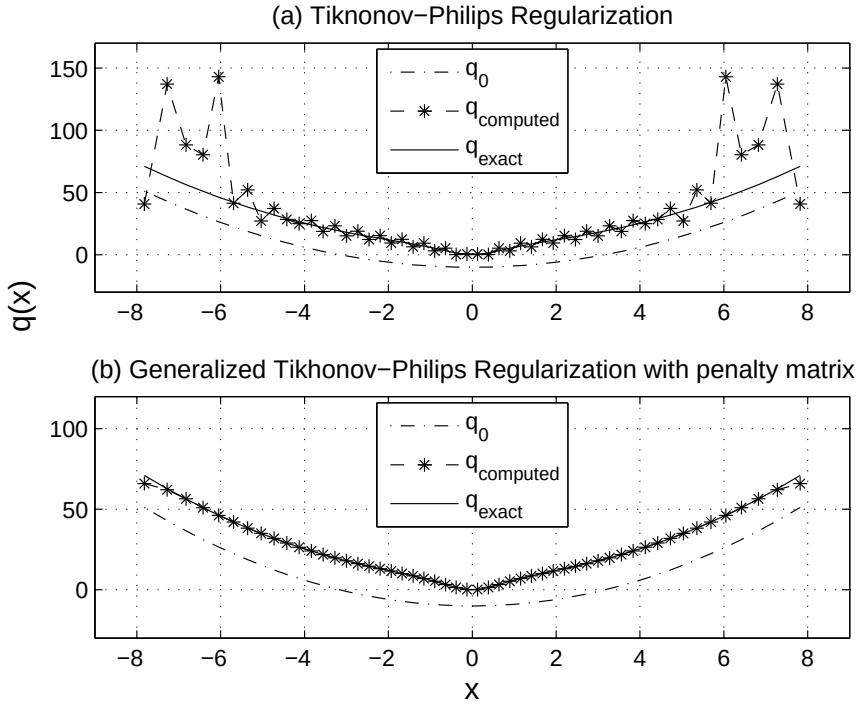

Figure 4.19: Effect of the penalty matrix in the generalized Tikhonov-Phlips scheme for anharmonic oscillator with $a = 10$, $b = 1$.

only the term L which is called penalty (or regularization) matrix. For our problem, the second method gives more better results especially in the unharmonic oscillator example. We demonstrate the effect of this matrix in Figure 4.19. Here we use second order differentiation matrix generated by Hermite-pseudospectral method. We obtain very good improvement around boundary in most cases.

The computational implementation for the determination of the regularization parameters in both L-Curve and generalized cross validation methods we use the regularization toolbax [35] with some modifications.

All algorithms in this thesis are implemented in Matlab program.

CHAPTER 5

CONCLUSION

Two algorithms based on Fourier and Hermite pseudospectral methods, respectively, have been presented for the first time to solve some singular inverse Sturm-Liouville systems. Numerical results suggest that a regularization is necessary so that the algorithms are incorporated with the Tikhonov-Philips regularization techniques. By this way we overcome considerably the numerical shortages resulting from the ill-conditioned structure of the singular problem.

It is noteworthy to point out some difficulties in the inverse problem for Sturm-Liouville systems. Firstly, the analysis of errors is not well-developed even in the regular case. Unlike the direct problem, in which the potential function is given analytically and the main error comes from the discretization method, inverse problem has many error sources. First of all we have only a finite number of eigenvalues whereas the reconstruction of the potential requires the complete spectrum. Moreover, the available eigenvalues are not exact in most cases. Thus, we are attempting to determine the potential from an incomplete and approximate set of eigenvalues. Especially, errors in higher indexed eigenvalues have a serious effect in the inverse computation. On the other hand, iterative methods need the computation of the spectrum in a numerical sense. Therefore error sources in the direct problem are also encountered and play a serious role in the inverse computation. In this thesis we aim to reduce this effect by selecting the pseudospectral methods in the direct computation of the eigenvalues [1].

Secondly, our main obstacle seems to be the ill-conditioned structure of the inverse problems under consideration. Although the regularization cures significantly the ill-

posedness, extra error sources come from the regularization parts of the algorithm as well. Especially, the lack of exact Jacobian matrix effects so much the accuracy since it is calculated numerically in each iteration step by Newton method. To reduce this error we evaluate the Jacobian for each modified potential starting from the carefully chosen initial one. This process is not necessary in regular inverse Sturm-Liouville problems.

The infinite interval in the second algorithm has been replaced by a finite one in a natural way. To be specific, the number of given eigenvalues automatically determines the degree of Hermite polynomials. That is, the algorithm assumes the roots of those Hermite polynomials as the nodal points. On the other hand, the size l of the truncated interval in the first algorithm is selected as an input parameter [73]. Since better results are expected as l increases, we increase accordingly the number of eigenvalues to this end.

Moreover, the first algorithm employs equally spaced nodes in the discretization while the second is based on the non-uniform grid suggested by the roots of Hermite polynomials in question. As is well known, the roots of the Hermite polynomials are clustered in the near vicinity of the origin and spread further. This phenomenon helps us to explain the insufficient results around the boundaries. Despite of this unwelcome event the second algorithm provides more satisfactory determination than the first algorithm in which the density of the evenly spaced nodes depends also on the number of used eigenvalues. The restriction on the available number of eigenvalues does not allow us to choose the mesh length as small as possible.

Furthermore, the selection of the initial potential and the determination of the regularization parameter have vital roles in the reconstruction algorithms. In most examples zero potential does not give convergent results. We need to supply good initial potential, which is sufficiently close to the exact potential, according to the theory of Newton methods [22]. The selection of the initial potential also effects the number of iteration number to reach the desired accuracy.

We propose noise-free parameter selection methods, namely L-curve and generalized cross validation, to determine the regularization parameter. When we try to determine regularization parameter by hand it is hard to take these parameter under control in

each iteration step. Thus it is possible to give regularization parameter at first iteration and we use it along all iterations. But parameter choice rules enable us to determine this parameter in each iteration automatically. We present this parameter determination picture by Fourier pseudospectral method with harmonic oscillator example in Table 5.1 and Figure 5.1. Initial potential ($q_0 = 0$), number of used eigenvalues ($n = 19$), truncation parameter ($l = 8$) and maximum iteration number ($N_{max} = 50$) are same in all figures and table. In Figure 5.1a-b we use generalized cross validation method to determine the regularization parameter. On the other hand, we give regularization parameter by hand after a few experiments to get the results in Figure 5.1c-d. It can be seen from the Table 5.1 that regularization parameter selection method by generalized cross validation gives more better results than that of by hand. Moreover, Figure 5.1b-d shows generalized cross validation reaches the desired accuracy with 8 iteration whereas it is not possible to reach the same accuracy during 50 iterations in the case for which regularization parameter is given by hand.

Table 5.1: Relative errors for harmonic oscillator potential at grid points

$l = 8, \quad n = 19$			
j	x_j	GCV	By Hand
1	-7.59	3.64×10^{-1}	4.44×10^{-1}
3	-6.77	2.69×10^{-2}	2.04×10^{-1}
5	-5.95	2.99×10^{-3}	1.37×10^{-2}
7	-5.13	1.05×10^{-4}	2.16×10^{-2}
9	-4.31	6.19×10^{-6}	1.07×10^{-2}
11	-3.49	1.15×10^{-6}	8.25×10^{-4}
13	-2.67	1.34×10^{-7}	8.14×10^{-3}
15	-1.85	4.68×10^{-7}	1.43×10^{-2}
17	-1.03	8.47×10^{-7}	3.79×10^{-2}
19	-0.21	1.22×10^{-5}	7.13×10^{-1}

Our research has a potential extension in the near future to singular problems on the half line and on a finite interval. Algorithms for solving related inverse problems may be constructed along the same line by using pseudospectral methods with Laguerre and Jacobi polynomials, respectively.

Additionally, the inverse Sturm-Liouville problem can be extended to higher dimensions. Sturm-Liouville equation of the Schrödinger form has the following two-dimensional analogue on $\mathbb{R}^2$

$$[-\Delta + q(x,y)]\, u = \lambda u, \qquad u \in L_2(\mathbb{R}^2) \tag{5.1}$$

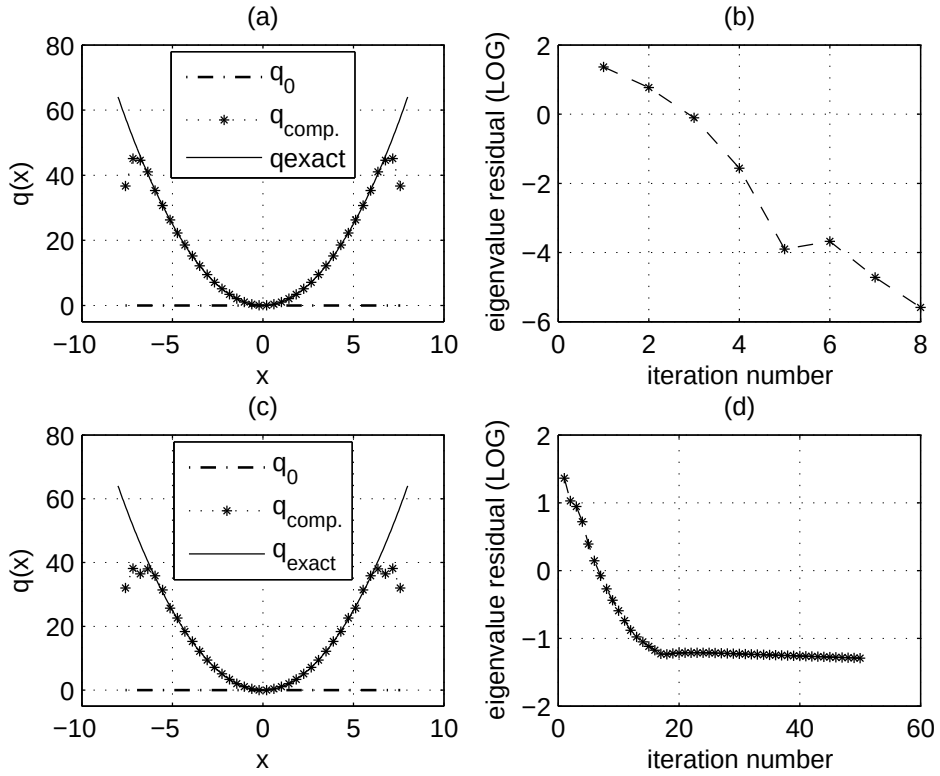

Figure 5.1: Reconstructed potential and convergence of eigenvalue residual with regularization parameter given by generalized cross validation rule (a-b), by hand (c-d) for harmonic oscillator example using Fourier pseudospectral method.

in which the wavefunction $u(x,y)$ satisfies the condition $\lim_{\|r\|\to\infty} u(r) = 0$, $r = (x,y)$, $x,y \in (-\infty,\infty)$ and Δ is the well-known Laplace's operator, i.e., $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$. The computation of eigenvalues λ in (5.1) for a given potential function $q(x,y)$ can be handled over a sufficiently large finite rectangular region Ω, obtained by truncating the domain of the independent variables x and y, i.e., $x \in [-l,l]$, $y \in [-m,m]$, subject to Dirichlet or Neumann boundary conditions [75, 76]. On the other hand, inverse problem in two-dimensional case deals with the recovering process of the potential from the knowledge of eigenvalues and corresponding wavefunctions. In contrast to one-dimensional inverse problem, higher dimensional version has few known results. It is known that the potential, which is symmetric with respect to the mid lines of the rectangle, can be reconstructed from the eigenvalues of (5.1) over rectangular region Ω with Dirichlet boundary conditions [46]. Thus we are planning to use truncation over both independent variables to built an algorithm which recovers the symmetric potentials from the given eigenvalues over a square region.

REFERENCES

[1] Alici, H. *A general pseudospectral formulation of a class of Sturm-Liouville Systems*. PhD thesis, Dept. of Math., Middle East Technical University, 2010.

[2] Ambartsumyan, V. A. Über aine frage der eignwerttheorie. *Z. Phys. 53* (1929), 690–695.

[3] Andrew, A. L. Asymptotic correction of Numerov's eigenvalue estimates with natural boundary conditions. *J. Comp. Appl. Math. 125* (2000), 359–366.

[4] Andrew, A. L. Asymptotic correction of more Sturm-Liouville eigenvalue estimates. *BIT 43* (2003), 485–503.

[5] Andrew, A. L. Numerical solution of inverse Sturm-Liouville problems. *ANZIAM J. 45(E)* (2004), C326–C337.

[6] Andrew, A. L. Numerov's method for inverse Sturm-Liouville problems. *Inverse Problems 21* (2005), 223–238.

[7] Andrew, A. L. Computing Sturm-Liouville potentials from two spectra. *Inverse Problems 22* (2006), 2069–2081.

[8] Andrew, A. L., and Paine, J. W. Correction of Numerov's eigenvalue estimates. *Numer. Math. 47* (1985), 289–300.

[9] Bailey, P. B., Everitt, W., and Zettl, A. The SLEIGN2 Sturm-Liouville code. *ACM Trans. Math. Software 21* (2001), 143–192.

[10] Bailey, P. B., Everitt, W. N., and Zettl, A. Computing eigenvalues of singular Sturm-Liouville problems. *Results in Mathematics 20* (1991), 391–423.

[11] Bakushinsky, A. B. The problem of the convergence of the iteratively regularized gauss-newton method. *Computational Mathematics and Mathematical Physics 32* (1992), 1353–1359.

[12] Bakushinsky, A. B., and Kokurin, M. Y. *Iterative methods for approximate solution of inverse problems*. Mathematics and its Applications. Springer, Dordrecht, 2004.

[13] Biswas, S. N., Datta, K., Saxena, P. K., Srivastava, P. K., and Varma, V. S. Eigenvalue of λx^{2m} anharmonic oscillators. *J. Math. Phys. 14* (1973), 1190–1195.

[14] Blaschke-Kaltenbacher, B., Neubauer, A., and Scherzer, O. On convergence rates for iteratively regularized gauss-newton method. *IMA J. Numer. Anal. 17* (1997), 421–436.

[15] Borg, G. Eine umkehrung der Sturm-Liouville eigenwertaufgabe. *Acta Math. 76* (1946), 1–96.

[16] Boyd, J. P. *Chebyshev and Fourier Spectral Methods*, 2nd ed. Dover Publications Inc., Mineola, NY, 2001.

[17] Brown, B. M., Samko, V. S., Knowles, I. W., and Marletta, M. Inverse spectral problem for the Sturm-Liouville equation. *Inverse Problems 19* (2003), 235–252.

[18] Browne, P., and Sleeman, B. Inverse nodal problem for sturm-liouville equation with eigenparameter dependent boundary conditions. *Inverse Problems 12* (1996), 377–381.

[19] Chadan, K., Colton, D., Päivärinta, L., and Rundell, W. *An introduction to Inverse Scattering and Inverse Spectral Problems*. Siam, Philadelphia, 1997.

[20] Coddington, E. A., and Levinson, N. *Theory of Ordinary Differential Equations*. McGraw-Hill, New York, 1955.

[21] Dahlberg, B. E. J., and Trubowitz, E. The inverse sturm liouville problem:III. *Comm. Pure. Appl. Math. 37* (1984), 255–267.

[22] Deuflhard, P. *Newton methods for nonlinear problems: Affine invariance and adaptive algorithms.* Springer-Verlag, Berlin, 2004.

[23] Engl, H. W., Hanke, M., and Neubauer, A. *Regularization of Inverse Problems*, vol. 375 of *Mathematics and Its Applications*. Kluwer Academic Publishers, Dordrecht, Boston, London, 1996.

[24] Fabiano, R. H., Knobel, R., and Lowe, B. D. A finite difference algorithm for an inverse Sturm-Liouville problem. *Ima J. Numer. Anal. 15* (1995), 75–88.

[25] Feng, X. Y. A solution of the inverse nodal problem. *Inverse Problems 13* (1997), 203–213.

[26] Freiling, G., and Yurko, V. *Inverse Sturm Liouville Problems and Their Applications*. Nova Science Publishers, Inc., Huntington, New York, 2001.

[27] Funaro, D. *Polynomial Aproximation of Differential Equations*. Springer Verlag, Berlin, 1992.

[28] Gel'fand, I. M., and Levitan, B. M. On the determination of a differential equation from its spectral function. *Trans. Amer. Math. Soc. 1* (1955), 253–304.

[29] Ghelardoni, P. Approximations of Sturm-Liouville eigenvalues using boundary value methods. *Applied Numerical Mathematics 23* (1997), 311–325.

[30] Golub, G. Heath, M., and Wahba, G. Generalized cross validation as a method for choosing a good ridge parameter. *Technometrics 21* (1979), 215–223.

[31] Hald, O., and McLaughlin, J. Solutions of inverse nodal problems. *Inverse Problems 5* (1989), 307–347.

[32] Hald, O. H. The inverse Sturm-Liouville problem with symmetric potentials. *Acta Math. 141* (1978), 263–291.

[33] Hanke, M. Regularization with differential operators. an iterative approach. *Numerical Functional Analysis and Optimization 13* (1992), 523–540.

[34] Hanke, M. A regularization Levenberg-Marguardt scheme, with application to inverse groundwater filtration problems. *Inverse Problems 13* (1997), 79–95.

[35] Hansen, P. C. Regularization Tools:A matlab package for analysis and solution of discrete ill-posed problems. *Numerical Algorithms 6* (1994), 1–35.

[36] Hansen, P. C. The l-curve and its use in the numerical treatment of inverse problems. In *In Computational Inverse Problems in Electrocardiology, ed. P. Johnston, Advances in Computational Bioengineering* (2000), WIT Press, pp. 119–142.

[37] Hochstadt, H., and Lieberman, B. An inverse Sturm-Liouville problem with mixed given data. *Siam J. Appl. Math. 34* (1976), 676–680.

[38] Isaacson, E., McKean, H., and Trubowitz, E. The inverse Sturm-Liouville problems II. *Comm. Pure. Appl. Math. 37* (1984), 1–11.

[39] Isaacson, E., and Trubowitz, E. The inverse Sturm-Liouville problems I. *Comm. Pure. Appl. Math. 36* (1983), 767–783.

[40] Jin, Q., and Tautenhahn, U. On the discrepancy principle for some Newton type methods for solving nonlinear inverse problems. *Numerische Mathematik 111* (2009), 509–558.

[41] Kaltenbacher, B. Some newton-type methods for the regularization of nonlinear ill-posed problems. *Inverse Problems 13* (1997), 729–753.

[42] Kammanee, A., and Böckmann, C. Determination of partially known Sturm-Liouville potentials. *Appl. Math. Comput. 204* (2008), 928–937.

[43] Kammanee, A., and Böckmann, C. Boundary value method for inverse Sturm-Liouville problems. *Appl. Math. Comput. 214* (2009), 342–352.

[44] Kirsch, A. *An introduction to the mathematical theory of inverse problems.*, vol. 120 of *Applied Mathematical Sciences*. Springer, Berlin, 1996.

[45] Kirsche, A., and Böckmann, C. Pade iteration method for regularization. *Appl. Math. Comput. 180* (2006), 648–663.

[46] Knobel, R., and McLaughlin, J. A reconstruction method for a two-dimensional inverse eigenvalue problem. *Z. Angew. Math. Phys. 45* (1994), 794–826.

[47] Koyunbakan, H., and Panakhov, E. A uniqueness theorem for inverse nodal problem. *Inverse Problems in Science and Engineering 15:6* (2007), 517–523.

[48] Ledoux, V., Van Daele, M., and Vanden Berghe, G. MATSLISE: A matlab package for the numerical solution of Sturm-Liouville and Schrödinger equations. *ACM Trans. Math. Software 31* (2005), 532–554.

[49] Levinson, N. The inverse Sturm-Liouville problem. *Math. Tidsskr B 25* (1949), 25–30.

[50] Levitan, B. M. *Inverse Sturm Liouville Problems*. VNU Science Press, Utrecht, 1987. (Translated from the Russian by O Efimov).

[51] Marchenko, V. A. Concerning the theory of a differential operator of second order. *Dokl. Akad. Nauk. SSR 72* (1950), 457–470.

[52] Marti, J. T. Small potential corrections for the discrete eigenvalues of the Sturm-Liouville problem. *Numer. Math. 57* (1990), 51–62.

[53] McLaughlin, J. Inverse spectral theory using nodal points as data - a uniqueness result. *Journal of Differential Equations 73* (1988), 354–362.

[54] Nashed, M. Z. *A new approach to classification and regularization of illposed operator equations*, vol. 4 of *In: H.W. Engl C.W. Groetsch (eds.), Inverse and Ill-posed Problems*. Academic Press, Orlando, 1987.

[55] Nashed, M. Z., and Chen, X. Convergence of newton-like methods for singular operator equations using outer inverses. *Numer. Math. 66* (1993), 235–257.

[56] Neher, M. Enclosing solutions of an inverse sturm-liouville problem with finite data. *Computing 53* (1994), 379–395.

[57] Neher, M. Enclosing solutions of an inverse sturm-liouville problem for an impedance. *Journal of Universal Computer Science 4* (1998), 178–192.

[58] Niessen, H. D., and Zettl, A. Singular Sturm-Liouville problems: the friedrichs extension and comparison of eigenvalues. *Proc. London Math. Soc. 64* (1992), 545–578.

[59] Paine, J. A numerical method for the inverse Sturm-Liouville problems. *SIAM J. Sci. Stat. Comput. 5* (1984), 149–156.

[60] Paine, J. W., de Hoog, F. R., and Anderssen, R. S. On the correction of finite difference eigenvalue approximations for Sturm-Liouville problems. *Computing 26* (1981), 123–139.

[61] Pirovino, M. H. The inverse Sturm-Liouville problem and finite differences. Tech. Rep. 93-04, Seminar für angewandte Mathematik, May 1993.

[62] Pöschel, J., and Trubowitz, E. *Inverse Spectral Theory*. Academic Press, London, 1987.

[63] Pruess, S., and Fulton, C. T. Mathematical software for Sturm-Liouville problems. *ACM Trans. Math. Software 19* (1993), 360–376.

[64] Pryce, J. D. *Numerical Solution of Sturm-Liouville Problems*. Oxford University Press, 1993.

[65] Pryce, J. D., and Marletta, M. Automatic solution of Sturm-Liouville problems using the pruess method. *J. Comput. and Appl. Math. 39* (1992), 57–78.

[66] Rafler, M., and Böckmann, C. Reconstruction method for inverse Sturm-Liouville problems with discontinuous potentials. *Inverse Problems 23* (2007), 933–946.

[67] Rieder, A. On convergence rates of inexact newton regularizations. *Numer. Math. 88* (2001), 347–356.

[68] Röhrl, N. A least-squares functional for solving inverse Sturm-Liouville problems. *Inverse Problems 21* (2005), 2009–2017.

[69] Rundell, W., and Sack, P. E. Reconstruction techniques for classical inverse Sturm-Liouville problems. *Mathematics of Computation 58 (197)* (1992), 161–183.

[70] Rundell, W., and Sack, P. E. The reconstruction techniques of inverse Sturm-Liouville operators. *Inverse Problems 8* (1992), 457–482.

[71] Sack, P. E. An iterative method for the inverse dirichlet problem. *Inverse Problems 4* (1988), 1005–1069.

[72] Şuhubi, E. S. *Functional Analysis*. Kluwer Academic, Dordrecht/Boston/London, 2003.

[73] Taşeli, H. Accurate numerical bounds for the spectral points of singular Sturm Liouville problems over $-\infty < x < \infty$. *J. Comput. Appl. Math. 115* (2000), 535–546.

[74] Taşeli, H., and Alici, H. The scaled Hermite-Weber basis in the spectral and pseudospectral pictures. *J. Math. Chem. 38* (2005), 367–378.

[75] Taşeli, H., and Eid, R. Converging bounds for the eigenvalues of multiminima potentials in two-dimensional space. *J. Phys. A: Math. Gen. 29* (1996), 6967–6982.

[76] Taşeli, H., and Eid, R. Eigenvalues of the two-dimensional Schrödinger equation with nonseperable potentials. *International Journal of Quantum Chemistry 59* (1996), 183–201.

[77] Titchmarsh, E. C. *Eigenfunction Expansions Associated with Second Order Differential Equations:Part I*. Clarendon Press, Oxford, 1962.

[78] Vogel, C. *Computational Methods for Inverse Problems*. SIAM, Philadelphia, 2002.

[79] Weidemann, J. A. C., and Reddy, S. C. A matlab differentiation matrix suit. *ACM T. Math. Software 26* (2000), 465–519.

[80] Welfert, B. D. Generation of pseudospectral differentiation matrices I. *SIAM J. Numer. Anal. 34* (1997), 1640–1657.

VITA

PERSONAL INFORMATION

Surname, Name	ALTUNDAĞ, Hüseyin
Nationality	Republic of Turkey
Date and Place of Birth	10.06.1977, Kırıkkale
Marital Status	Married
Phone Number	+90 532 468 69 91
E-mail Adress	altundagh@gmail.com

EDUCATION

Degree	Institution	Year of Graduation
Ph. D.	METU, Mathematics Department	2010
M. Sc.	METU, Mathematics Department	2005
B. Sc.	Ankara University, Mathematics Department	1998

WORK EXPERIENCE

Year	Place	Enrollment
2002-2010	METU, Mathematics Department	Research Assistant
2005-2006	Potsdam University	Guest Researcher
2000-2002	İYTE, Mathematics Department	Research Assistant

FOREIGN LANGUAGE

English

FIELD OF STUDY

Numerical Solutions of ODE's, Pseudospectral Methods, Inverse Problems, Regularization Techniques.