8-26-2011

Proximal point methods for inverse problems

Marc Paulhamus

Proximal Point Methods for Inverse Problems

by

Marc Paulhamus

A thesis submitted in partial fulfillment of
the requirements for the degree of
Master of Science in Applied Mathematics
from the School of Mathematical Sciences
Rochester Institute of Technology

26 August 2011

Advisor:	Dr. Akhtar Khan
Committee members:	Dr. Patricia Clark
	Dr. Baasansuren Jadamba
	Dr. Miguel Sama

Dedicated to my parents

Larry and Connie Paulhamus
with deep love.

Proximal Point Methods for Inverse Problems

by

Marc Paulhamus

Abstract

Numerous mathematical models in applied mathematics can be expressed as a partial differential equation involving certain coefficients. These coefficients are known and they describe some physical properties of the model. The direct problem in this context is to solve the partial differential equation. By contrast, an inverse problem asks for the identification of the variable coefficients when a certain measurement of a solution of the partial differential equation is available. One of the most commonly used approaches for solving this inverse problem is by posing a constrained minimization problem which can be written as a variational inequality.
This paper investigates the inverse problem of identifying certain material parameters in the fourth-order partial differential equations representing the beam and plate models. This inverse problem has attracted a great deal of attention in recent years and has found numerous applications. Since the numerical treatment of the fourth-order problems is rather challenging, the first part of the paper describes in detail the finite element approach for solving the direct problem. The inverse problem is solved by posing an optimization problem whose solution is an approximation of the parameters sought. The optimization problem is solved by gradient based approaches, and in this setting, the most challenging aspect is the computations of the gradient of the objective function. We present a detailed treatment of three approaches to compute the gradient, namely, the so-called adjoint method, adjoint stiffness based approach, and the classical gradient computation. We also present a comparison among these different ways of gradient computation. We use different proximal point methods to solve the inverse problem. It is know that proximal point method is a regularization method which has a significantly different behavior than the well-know Tikhonov regularization method. We present a detailed comparative analysis of the numerical efficiency of several proximal point methods.

Acknowledgement

Words cannot express my gratitude for my advisor, Dr. Akhtar Khan for his professional advice and assistance in reviewing this thesis. He genuinely cares for his students and his love of mathematics makes for an astounding combination to lead his student to great accomplishments. Bless him and his family.

I would like to thank the School of Mathematical Sciences at RIT. The faculty here is truly exceptional. They go beyond the expectation of sharing their knowledge by demonstrating how mathematics should be studied at a higher level.

Lastly, the encouragement of my parents cannot go unnoticed. They have been there for me emotionally, morally, and financially. It makes a world of a difference knowing your parents are behind you.

Special thanks to my committee members: Prof. Patricia Clark, Dr. Baasansuren Jadamba, Dr. Miguel Sama, and the director of graduate programs, Prof. Tamas Wiandt.

Contents

List of Figures **vii**

List of Tables **x**

1 Introduction to Inverse Problems **1**

1.1 Inverse Problems 1

1.2 Optimization Formulation 2

1.3 Organization 3

2 Fourth-Order Boundary Value Problems **4**

2.1 The Weak Form 4

2.2 The Finite Element Method 5

2.3 Implementation Issues 12

2.3.1 Load Vector 12

2.3.2 Stiffness Matrix 14

2.4 Numerical Experiments 20

3 Optimization Formulation of Inverse Problems **23**

3.1 Problem Formulation 23

3.2 Optimization Formulation: Finite Dimensional Case 27

3.3 Output Least-Squares (OLS) 27

3.4 Modified Output Least-Squares (MOLS) 30

3.5 Regularization 32

4 Identification by Derivative Free Methods **34**

4.1 Nelder-Mead Method 34

4.2 Nelder-Mead Algorithm 35
4.3 Numerical Results 36

5 Computation of the Derivatives 39
5.1 Adjoint Stiffness Matrix Based Approach 39

6 Proximal Point Method 66
6.1 Optimization Formulation 66
6.2 Test Examples 68
6.3 Proximal-Like Methods Using Least Squares 69
6.4 Proximal-like Methods Using φ-Divergence 75
6.5 Proximal-like Methods Using Bregman Functions 81
6.6 Proximal-like Methods Using Modified φ-Divergence 88
6.7 Han Proximal-Point Method 94
6.8 Li-Yuan Proximal Point Method 99

7 Comparative Performance Analysis 104
7.1 Numerical Results for Example 1 104
7.2 Numerical Results for Example 2 108
7.3 Numerical Results for Example 3 112
7.4 Numerical Results for Example 4 115

Bibliography 118

List of Figures

2.1 Basis Function ϕ_j 7
2.2 Basis Function ψ_j 8
2.3 Example 1 20
2.4 Example 2 21
2.5 Example 3 21
2.6 Example 4 22

4.1 Example 1 using Nelder-Mead Simplex Method 36
4.2 Example 2 using Nelder-Mead Simplex Method 37
4.3 Example 3 using Nelder-Mead Simplex Method 37
4.4 Example 4 using Nelder-Mead Simplex Method 38

5.1 Basis function ϕ_j 41
5.2 Basis function ψ_j 42
5.3 Basis function a_0 42
5.4 Basis function a_1 42
5.5 Basis function a_2 44
5.6 Basis function a_3 45
5.7 Basis function a_{n-1} 47
5.8 Basis function a_n 48
5.9 Basis functions a_{n+1} 49

6.1 Example 1: Coefficient by Hager-Zhang Method using Least Squares 71
6.2 Example 1: Solution by Hager-Zhang Method using Least Squares 71
6.3 Example 2: Coefficient by Hager-Zhang Method using Least Squares 72
6.4 Example 2: Solution by Hager-Zhang Method using Least Squares 72

6.5 Example 3: Coefficient by Hager-Zhang Method using Least Squares 73
6.6 Example 3: Solution by Hager-Zhang Method using Least Squares 73
6.7 Example 4: Coefficient by Hager-Zhang Method using Least Squares 74
6.8 Example 4: Solution by Hager-Zhang Method using Least Squares 74
6.9 Example 1: Coefficient by Hager-Zhang Method using φ-divergence 77
6.10 Example 1: Solution by Hager-Zhang Method using φ-divergence 77
6.11 Example 2: Coefficient by Hager-Zhang Method using φ-divergence 78
6.12 Example 2: Solution by Hager-Zhang Method using φ-divergence 78
6.13 Example 3: Coefficient by Hager-Zhang Method using φ-divergence 79
6.14 Example 3: Solution by Hager-Zhang Method using φ-divergence 79
6.15 Example 4: Coefficient by Hager-Zhang Method using φ-divergence 80
6.16 Example 4: Solution by Hager-Zhang Method using φ-divergence 80
6.17 Example 1: Coefficient by Hager-Zhang Method using Bregman function . . . 84
6.18 Example 1: Solution by Hager-Zhang Method using Bregman function 84
6.19 Example 2: Coefficient by Hager-Zhang Method using Bregman function . . . 85
6.20 Example 2: Solution by Hager-Zhang Method using Bregman function 85
6.21 Example 3: Coefficient by Hager-Zhang Method using Bregman function . . . 86
6.22 Example 3: Solution by Hager-Zhang Method using Bregman function 86
6.23 Example 4: Coefficient by Hager-Zhang Method using Bregman function . . . 87
6.24 Example 4: Solution by Hager-Zhang Method using Bregman function 87
6.25 Example 1: Coefficient by Hager-Zhang Method using quadratic function . . . 90
6.26 Example 1: Solution by Hager-Zhang Method using quadratic function 90
6.27 Example 2: Coefficient by Hager-Zhang Method using quadratic function . . . 91
6.28 Example 2: Solution by Hager-Zhang Method using quadratic function 91
6.29 Example 3: Coefficient by Hager-Zhang Method using quadratic function . . . 92
6.30 Example 3: Solution by Hager-Zhang Method using quadratic function 92
6.31 Example 4: Coefficient by Hager-Zhang Method using quadratic function . . . 93
6.32 Example 4: Solution by Hager-Zhang Method using quadratic function 93
6.33 Example 1: Coefficient by Han Method 95
6.34 Example 1: Solution by Han Method 95
6.35 Example 2: Coefficient by Han Method 96
6.36 Example 2: Solution by Han Method 96
6.37 Example 3: Coefficient by Han Method 97

6.38 Example 3: Solution by Han Method 97
6.39 Example 4: Coefficient by Han Method 98
6.40 Example 4: Solution by Han Method 98
6.41 Example 1: Coefficient by Li-Yuan Method 100
6.42 Example 1: Solution by Li-Yuan Method 100
6.43 Example 2: Coefficient by Li-Yuan Method 101
6.44 Example 2: Solution by Li-Yuan Method 101
6.45 Example 3: Coefficient by Li-Yuan Method 102
6.46 Example 3: Solution by Li-Yuan Method 102
6.47 Example 4: Coefficient by Li Method 103
6.48 Example 4: Solution by Li-Yuan Method 103

List of Tables

7.1 Results of Example 1. 105
7.2 Example 1. Using Hager and Zhang-LS 106
7.3 Example 1. Using Hager and Zhang-φ 106
7.4 Example 1. Using Hager and Zhang-Bregman Function 107
7.5 Example 1 Using Hager and Zhang-Quadratic Function 107
7.6 New Results of Example 1. 108
7.7 Results of Example 2. 108
7.8 Example 2. Using Hager and Zhang-NR 109
7.9 Example 2. Using Hager and Zhang-LS 109
7.10 Example 2. Using Hager and Zhang-φ 110
7.11 Example 2. Using Hager and Zhang-Bregman Function 110
7.12 Example 2. Using Hager and Zhang-Quadratic Function 111
7.13 New Results of Example Two 111
7.14 Results of Example 3. 112
7.15 Example 3. Using Hager and Zhang-NR 112
7.16 Example 3. Using Hager and Zhang-LS 113
7.17 Example 3. Using Hager and Zhang-φ 113
7.18 Example 3. Using Hager and Zhang-Brgman Function 114
7.19 Example 3. Using Hager and Zhang-Quadratic Function 114
7.20 New Results of Example 3. 115
7.21 Results of Example Four 115
7.22 Example 4. Using Hager and Zhang-NR 116
7.23 Example 4. Using Hager and Zhang-LS 116
7.24 Example 4. Using Hager and Zhang-φ 117
7.25 Example 4. Using Hager and Zhang-Bregman Function 117

7.26 Example 4. Using Hager and Zhang-Quadratic 118
7.27 New Results of Example 4 118

Chapter 1

Introduction to Inverse Problems

This chapter gives a general description of inverse problems and introduces the specific inverse problem that is the subject of this thesis. We conclude this chapter by giving a detailed outline and organization of this thesis.

1.1 Inverse Problems

The field of inverse problems has grown tremendous interest in the realm of researchers. This is justified by the importance of the applications they lead to. With the advancement of fast computers and stable numerical methods, inverse problems are leading the way in medical imaging, computer vision, physics, and many other fields.

In this work, we deal with an inverse problem of coefficient identification in boundary value problems. In direct problems, we are given physical quantities (or the model parameters), and need to find the solution. On the other hand, in inverse problems, we have a measurement of the solution, the data, and the objective is to find the model parameters.

Our primary objective is to study the inverse problem of the identification of a variable coefficient in the beam equation. To be specific, we focus on the following static fourth-order boundary value problem in $\Omega = (0,1)$:

$$\begin{aligned} \left(a(x)u''\right)'' &= f(x), 0 < x < 1, &\quad (1.1a)\\ u(0) &= u'(0) = 0, &\quad (1.1b)\\ u(1) &= u'(1) = 0, &\quad (1.1c) \end{aligned}$$

where $a(x)$ is a variable coefficient and f is a suitable function.

The boundary conditions (1.1b)-(1.1c) are the so-called clamped boundary conditions. However, our approach can easily be carried over to other types of boundary conditions as well.
This inverse problem has attracted a great deal of attention in recent years and has found numerous applications. Some details can be found in [7], [10], [11], [21], [27], [28], [35], [38], [39], [40], [41], [42], [43], [44], [45], [46], [48] and the cited references therein.
Referring to (3.1), the goal of the direct problem for this BVP is to find $u(x)$, given that $a(x)$ and (f) are known. In the inverse problem, the goal is to find the coefficient $a(x)$ when a measurement z of the solution $u(x)$ is known.
Inverse problems are challenging primarily due to the fact that they are ill-posed. To explain this concept, we recall that a problem is well-prosed if it satisfies the following three conditions:

1. A solution exist.

2. The solution is unique.

3. The solution depends continuously on the data.

If one of the conditions is not met, then the problem is considered to be ill-posed. It can be shown that direct problems are well-posed, but inverse problems are ill posed.
If in (1.1a), we integrate both sides twice and solve for $a(x)$, we obtain

$$a(x) = \frac{1}{u''} \iint_{\Omega} f(x).$$

Clearly, the coefficient is not defined in the regions where $u'' = 0$.

1.2 Optimization Formulation

The coefficient $a(x)$ in (3.1) can be obtained by solving the BVP for the coefficient. However, it has been shown by explicit examples for the simpler BVPs that this approach is not very fruitful.
Therefore, instead of solving for $a(x)$ directly, a commonly adopted approach for solving inverse problems is to pose an equivalent optimization problem whose solution is an approximation of the coefficient to be identified. The idea is to minimize the norm of the difference between the computed solution and the measured solution. Several variants of this idea are available.

In the context of our problem, one possibility is that given a measurement z, the coefficient $a(x)$ should be chosen to minimize the output least-squares (OLS) functional

$$J(a) = \frac{1}{2}\|u(a) - z\|^2, \tag{1.2}$$

where $\|\cdot\|$ is a suitable norm and $u(x)$ is the solution obtained by solving the direct problem for the coefficient $a(x)$.

A common remedy to the ill-posedness is by using regularization. That is, instead of the OLS, we indeed solve the minimization problem

$$\min_{a\in\tilde{A}} \{J(a) + \varepsilon R(a)\}, \tag{1.3}$$

where $R(a)$ is called a regularization term, $\varepsilon > 0$ is the regularization parameter, and $\tilde{A}$ is the set of all feasible coefficients.

The variational inequality of finding $a^* \in \tilde{A}$

$$\left\langle J'(a^*) + R'(a), a - a^* \right\rangle \geq 0 \quad \forall a \in \tilde{A}, \tag{1.4}$$

then turns out to be the necessary optimality condition for the OLS optimization problem.

Other optimization formulations will be discussed in the following chapters.

1.3 Organization

The contents of this thesis are organized into seven chapters. In Chapter 2 we discuss the fourth-order boundary value problem into significant details. We describe the suitable function spaces in which the functions and the solution should reside. We derive the weak form associated to the boundary value problem. We develop a complete finite element based framework for obtaining a numerical solution. Implementation issues are also discussed in detail. Numerical examples are given to show the efficiency of the developed numerical approach. In Chapter 3 we pose the inverse problems as a minimization problem. Several results concerning the differentiability of the coefficient-to-solution map and the objective functional are given. In Chapter 4 we solve the inverse problem by using the Nelder-Mead method, an iterative derivative-free method. In order to use derivative based methods, the adjoint stiffness matrix based approach is developed in Chapter 5 for the numerical computation of the gradient of the objective functional. Chapter 6 employs several proximal point methods for the inverse problem. Each method is tested by means of several examples. A comparative study of the proximal point methods in terms of the over all computational cost involved and their numerical efficiency is given in Chapter 7.

Chapter 2

Fourth-Order Boundary Value Problems

In this chapter we describe the details of the fourth-order boundary value problem that is the theme of this thesis. We obtain the weak form of the BVP. The finite element method is used to discretize the weak form. Implementation issues are discussed. Several examples are given to show the performance of the finite element method.

2.1 The Weak Form

As already mentioned, our primary objective is to study the inverse problem of the identification of variable coefficients in the beam equation. To be specific, we focus on the following static fourth-order boundary value problem in $\Omega = (0,1)$:

$$
\begin{aligned}
\left(a(x)u''\right)'' &= f(x), 0 < x < 1, && \text{(2.1a)}\\
u(0) &= u'(0) = 0, && \text{(2.1b)}\\
u(1) &= u'(1) = 0, && \text{(2.1c)}
\end{aligned}
$$

where $a(x)$ is a variable coefficient and f is a suitable function.
The function space convenient for our setting is then defined by:

$$V = \left\{ u \in H^2(\Omega) |\; u(0) = u'(0) = u(1) = u'(1) = 0 \right\}.$$

To obtain the weak form of (2.1), we multiply (2.1a) by a test function $v \in V$,

$$\left(a(x)u''\right)'' v = fv.$$

Integrating over the interval $(0,1)$ yields

$$\int_0^1 \left(a(x)u''\right)'' v\,dx = \int_0^1 fv dx.$$

By performing integration by parts twice and using the boundary conditions, we obtain

$$\int_0^1 a(x)u''v''dx = \int_0^1 fvdx.$$

Since v is arbitrary, we have obtained

$$\left\langle a(x)u'', v''\right\rangle = \langle f, v\rangle\,, \quad \text{for all } v \in V, \tag{2.2}$$

where

$$\langle f, g\rangle = \int_0^1 fg\,dx.$$

Equation (2.2) is often referred to as the weak form or the variational form of (2.1).

2.2 The Finite Element Method

To define the finite element space, we start with a partition of Ω :

$$0 = x_0 < x_1 < \cdots < x_j < \cdots < x_N < x_{N+1} = 1.$$

We then define

$$I_j =]x_{j-1}, x_j[, \quad \text{for } j = 1, \ldots, N+1$$

and the corresponding step-length

$$h_j = x_j - x_{j-1}.$$

The finite element space V_h consists of elements v that satisfy the following three conditions:

- v and v' are continuous.
- v is a polynomial of degree 3 on each subinterval I_j.
- The boundary conditions (2.1b) and (2.1b) hold for v.

Since $V_h \subset V$, we can consider the following finite-dimensional weak form: Find $u_h \in V_h$ such that

$$\left\langle a(x)u_h'', v''\right\rangle = \langle f, v\rangle\,, \quad \text{for all } \; v \in V_h. \tag{2.3}$$

Since a three degree polynomial has four degrees of freedom, an element $v \in V_h$ on any interval I_j can be uniquely determined by four values, namely, $v(x_{j-1})$, $v(x_j)$, $v'(x_{j-1})$ and $v'(x_j)$. Therefore, at every point of the mesh, any $v \in V_h$ has two degrees of freedom, namely, the function value v and its derivative value v'. To define a bases for V_h we will define two basis functions for every node.
Let ϕ_{j-1} be the basic function that corresponds to $v(x_{j-1})$ satisfying:

$$\begin{aligned} v(x_{j-1}) &= 1, \\ v(x_j) &= 0, \\ v'(x_{j-1}) &= 0, \\ v'(x_j) &= 0. \end{aligned} \tag{2.4}$$

Since $\phi_{j-1} \in V_h$, it is a third degree polynomial, and hence its general form is,

$$\phi_{j-1}(x) = ax^3 + bx^2 + cx + d, \quad \text{where } 0 \neq a,b,c,d \in \mathbb{R}.$$

Using the constraints (2.4), we obtain the following system of equations:

$$\begin{pmatrix} \phi_{j-1}(x_{j-1}) \\ \phi_{j-1}(x_j) \\ \phi'_{j-1}(x_{j-1}) \\ \phi'_{j-1}(x_j) \end{pmatrix} = \begin{pmatrix} ax_{j-1}^3 + bx_{j-1}^2 + cx_{j-1} + d \\ ax_j^3 + bx_j^2 + cx_j + d \\ 3ax_{j-1}^2 + bx_{j-1} + c \\ 3ax_j^2 + bx_j + c \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

The above system can be written as

$$\begin{pmatrix} x_{j-1}^3 & x_{j-1}^2 & x_{j-1} & 1 \\ x_j^3 & x_j^2 & x_j & 1 \\ 3x_{j-1}^2 & x_{j-1} & 1 & 0 \\ 3x_j^2 & x_j & 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

By solving this system, we get

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \frac{1}{h_j^3} \begin{pmatrix} 2 \\ -3(x_{j-1} + x_j) \\ 6x_{j-1}x_j \\ (x_j - 3x_{j-1})x_j^2 \end{pmatrix}$$

where $h_j = x_j - x_{j-1}$.

Consequently,

$$\phi_{j-1}(x) = \frac{1}{h_j^3}\left[2x^3 - 3(x_{j-1}+x_j)x^2 + 6x_{j-1}x_jx + (x_j - 3x_{j-1})x_j^2\right] \quad x \in I_j. \tag{2.5}$$

To get a general idea about the shape of the basis function, see Figure 2.1.

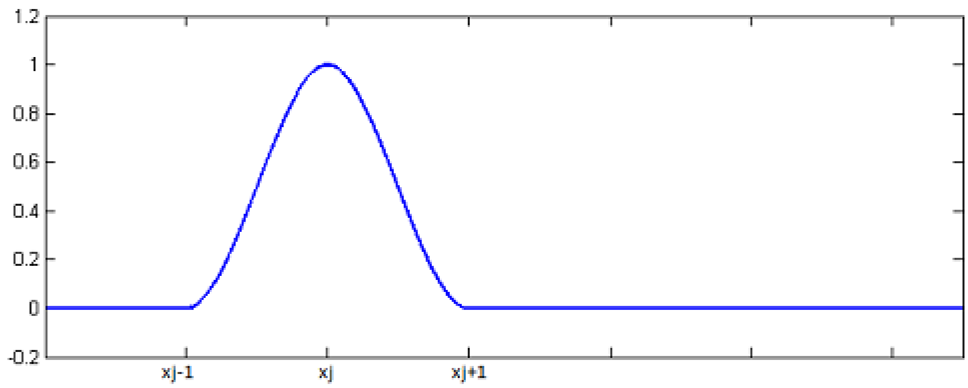


Figure 2.1: Basis Function ϕ_j.

Indeed this equation will represent the part of the basic function from x_j to x_{j+1} due to the conditions in (2.4). To get the part of the function from x_{j-1} to x_j, we will use the conditions:

$$\begin{aligned} v(x_{j-1}) &= 0, \\ v(x_j) &= 1, \\ v'(x_{j-1}) &= 0, \\ v'(x_j) &= 0. \end{aligned} \tag{2.6}$$

We obtain the following resulting system of equations

$$\phi_{j-1}(x) = \frac{1}{h_j^3}\left[-2x^3 + 3(x_{j-1}+x_j)x^2 - 6x_{j-1}x_jx + (3x_j - x_{j-1})x_{j-1}^2\right] \text{ for } x \in I_j. \tag{2.7}$$

Using both the ϕ_{j-1} and ϕ_j, a description for ϕ_j can be given for all $x \in [0,1]$ and $j = 1,\ldots,N$

$$\phi_j(x) = \begin{cases} \frac{1}{h_j^3}\left[-2x^3 + 3(x_{j-1}+x_j)x^2 - 6x_{j-1}x_jx + (3x_j - x_{j-1})x_{j-1}^2\right] & x \in\ I_j \\ \frac{1}{h_{j+1}^3}\left[2x^3 - 3(x_j+x_{j+1})x^2 + 6x_jx_{j+1}x + (x_{j+1} - 3x_j)x_{j+1}^2\right] & x \in\ I_{j+1} \\ 0 & \text{otherwise.} \end{cases}$$

For the later use, we also compute the second derivative of ϕ_j for $j = 1,\ldots,N$

$$\phi_j''(x) = \begin{cases} \frac{1}{h_j^3}\left[-12x + 6(x_{j-1} + x_j)\right] & x \in I_j \\ \frac{1}{h_{j+1}^3}\left[12x - 6(x_j + x_{j+1})\right] & x \in I_{j+1} \\ 0 & \text{otherwise.} \end{cases} \tag{2.8}$$

Let the basis function that corresponds to $v'(x_{j-1})$ be ψ_j. Using the conditions from (2.9) and (2.11), we can expect to get a picture like shown in Figure 2.2.

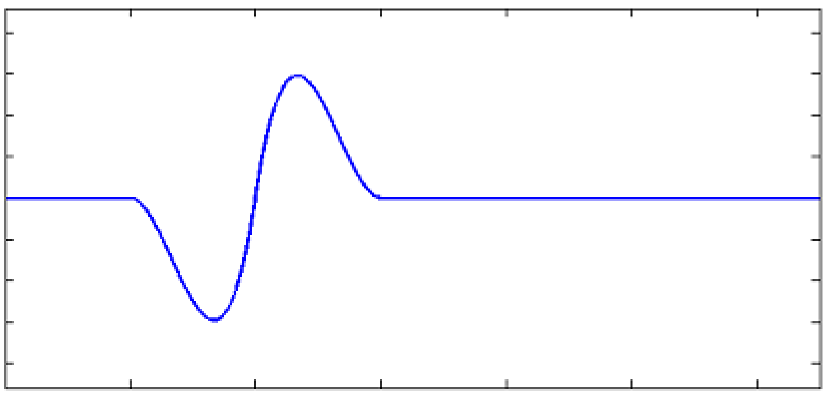


Figure 2.2: Basis Function ψ_j

We will need to use the conditions from (2.9):

$$\begin{aligned} v(x_{j-1}) &= 0, \\ v(x_j) &= 0, \\ v'(x_{j-1}) &= 1, \\ v'(x_j) &= 0. \end{aligned} \tag{2.9}$$

The resulting system of equations reads:

$$\begin{pmatrix} \psi_{j-1}(x_{j-1}) \\ \psi_{j-1}(x_j) \\ \psi'_{j-1}(x_{j-1}) \\ \psi'_{j-1}(x_j) \end{pmatrix} = \begin{pmatrix} ax_{j-1}^3 + bx_{j-1}^2 + cx_{j-1} + d \\ ax_j^3 + bx_j^2 + cx_j + d \\ 3ax_{j-1}^2 + bx_{j-1} + c \\ 3ax_j^2 + bx_j + c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}.$$

Therefore,

$$\begin{pmatrix} x_{j-1}^3 & x_{j-1}^2 & x_{j-1} & 1 \\ x_j^3 & x_j^2 & x_j & 1 \\ 3x_{j-1}^2 & x_{j-1} & 1 & 0 \\ 3x_j^2 & x_j & 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}.$$

Solving the above system, we get

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \frac{1}{h_j^2} \begin{pmatrix} 1 \\ -(x_{j-1}+x_j) \\ x_j(2x_{j-1}+x_j) \\ -x_{j-1}x_j^2 \end{pmatrix}$$

where $h_j = x_j - x_{j-1}$.
Consequently

$$\psi_{j-1}(x) = \frac{1}{h_j^2}\left[x^3 - (x_{j-1}+2x_j)x^2 + x_j(2x_{j-1}+x_j)x - x_{j-1}x_j^2\right] \text{ for } x \in I_j. \tag{2.10}$$

This equation will represent the part of the basic function in Figure 2.2, from x_j to x_{j+1} due to the conditions in (2.9). To get the part of the function from x_{j-1} to x_j in Figure 2.2, we will use the conditions:

$$\begin{aligned} v(x_{j-1}) &= 0, \\ v(x_j) &= 0, \\ v'(x_{j-1}) &= 0, \\ v'(x_j) &= 1. \end{aligned} \tag{2.11}$$

This leads to

$$\psi_j(x) = \frac{1}{h_j^2}\left[x^3 - (2x_{j-1}+x_j)x^2 + x_{j-1}(x_{j-1}+2x_j)x - x_{j-1}^2 x_j\right] \text{ for } x \in I_j \tag{2.12}$$

Using both the ψ_{j-1} and ψ_j, a description for ψ_j can be given for all $x \in [0,1]$ and $j = 1,\dots,N$

$$\psi_j(x) = \begin{cases} \frac{1}{h_j^2}\left[x^3 - (2x_{j-1}+x_j)x^2 + x_{j-1}(x_{j-1}+2x_j)x - x_{j-1}^2 x_j\right] & x \in I_j \\ \frac{1}{h_{j+1}^2}\left[x^3 - (x_j+2x_{j+1})x^2 + x_{j+1}(2x_j+x_{j+1})x - x_j x_{j+1}^2\right] & x \in I_{j+1} \\ 0 & \text{otherwise.} \end{cases}$$

The second derivative will be of importance to me later, so we have derive the second derivative of ψ_j for $j = 1, \ldots, N$

$$\psi_j''(x) = \begin{cases} \frac{1}{h_j^2}\left[6x - 2(2x_{j-1} + x_j)\right] & x \in I_j \\ \frac{1}{h_{j+1}^2}\left[6x - 2(x_j + 2x_{j+1})\right] & x \in I_{j+1} \\ 0 & \text{otherwise.} \end{cases} \tag{2.13}$$

We have now constructed a set of basis functions $\{\phi_1, \ldots, \phi_N, \psi_1, \ldots, \psi_N\}$ or $\{\phi_j, \psi_j\}_j^N$ for V_h. By the definition of V_h, any element $v \in V_h$ can be uniquely written as:

$$v = \sum_{j=1}^{N} [v_j \phi_j + \hat{v}_j \psi_j], \tag{2.14}$$

where $v_j = v(x_j)$ and $\hat{v}_j = v'(x_j)$.
Let $u_h \in V_h$ be the solution of the finite-dimensional weak form. Using (2.14), we obtain

$$u_h = \sum_{j=1}^{N} [u_j \phi_j + \hat{u}_j \psi_j], \quad j = 1, \ldots, N. \tag{2.15}$$

To obtain a matrix form for the weak form we proceed as follows: By setting $v = \phi_j$ in (2.2), we get

$$\left\langle a(x) u_h'', \phi_j'' \right\rangle = \langle f, \phi_j \rangle,$$

which further implies that

$$\left\langle a(x) \sum_{j=1}^{N} \left[u_j \phi_j'' + \hat{u}_j \psi_j''\right], \phi_j'' \right\rangle = \langle f, \phi_j \rangle.$$

By using the linearity of the inner product, we obtain

$$\sum_{j=1}^{N} u_j \left\langle a(x) \phi_j'', \phi_i'' \right\rangle + \sum_{j=1}^{N} \hat{u}_j \left\langle a(x) \psi_j'', \phi_i'' \right\rangle = \langle f, \phi_i \rangle. \tag{2.16}$$

Analogously, by taking $v = \psi_j$, we obtain

$$\sum_{j=1}^{N} u_j \left\langle a \phi_j'', \psi_i'' \right\rangle + \sum_{j=1}^{N} \hat{u}_j \left\langle a \psi_j'', \psi_i'' \right\rangle = \langle f, \psi_i \rangle. \tag{2.17}$$

Equations (2.16) and (2.17) now give me a system of $2N$ equations in $2N$ unknowns, namely $\{u_1, \ldots, u_N, \hat{u}_1, \ldots, \hat{u}_N\}$.

We will now write this system in terms of a matrix equation. For $i, j = 1, \ldots, N$, we define $N \times N$ matrices A, B, and C by

$$\begin{aligned} A_{ij} &= \left\langle a(x)\phi_j'', \phi_i'' \right\rangle, \\ B_{ij} &= \left\langle a(x)\psi_j'', \phi_i'' \right\rangle, \\ C_{ij} &= \left\langle a(x)\psi_j'', \psi_i'' \right\rangle. \end{aligned}$$

Furthermore, defining the vectors $F_\phi, F_\psi \in \mathbb{R}^N$ by

$$\begin{aligned} F_\phi &= (\langle f, \phi_1 \rangle, \ldots, \langle f, \phi_N \rangle)^T \\ F_\psi &= (\langle f, \psi_1 \rangle, \ldots, \langle f, \psi_N \rangle)^T. \end{aligned}$$

Then $U \in \mathbb{R}^{2N}$ is given by

$$U = (u_1, \ldots, u_N, \hat{u}_1, \ldots, \hat{u}_N)^T.$$

From equations (2.16) and (2.17), we obtain the system,

$$KU = F$$

where the stiffness matrix K has the form

$$K = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix}$$

and the load vector F is given by

$$F = \begin{pmatrix} F_\phi \\ F_\psi \end{pmatrix}.$$

Notice that when $|i - j| > 1$ then from the definition of ϕ and ψ,

$$\phi_j'' \phi_j'' = \psi_j'' \psi_j'' = \phi_j'' \psi_j'' = 0 \text{ when } |i = j| > 1.$$

Therefore this leads to,

$$\left\langle a\phi_j'', \phi_j'' \right\rangle = \left\langle a\psi_j'', \psi_j'' \right\rangle = \left\langle a\phi_j'', \psi_j'' \right\rangle = 0 \text{ when } |i = j| > 1.$$

From this, it can be shown that the A, B, and C are tridiagonal.

2.3 Implementation Issues

Knowing how to write the fourth order boundary value problem as system of equations, we now switch to the implementation aspects. First task is to numerically approximate the integrals. We will do this by using Simpson's rule. When integrating over the interval $I_j = [x_{j-1}, x_j]$, Simpson's rule states,

$$\int_{x_{j-1}}^{x_j} f(x)dx = \frac{h_j}{6}[f(x_{j-1}) + 4f(x_{j-1/2}) + f(x_j)] \tag{2.18}$$

where $x_{j-1/2}$ is the midpoint of the interval I_j. Similarly, on I_{j+1},

$$\int_{x_j}^{x_{j+1}} f(x)dx = \frac{h_j}{6}[f(x_j) + 4f(x_{j+1/2}) + f(x_{j+1})] \tag{2.19}$$

where $x_{j+1/2}$ is the midpoint of the interval I_{j+1}.

2.3.1 Load Vector

We now construct the load vector, $F = (F_\phi, F_\psi)^T$ where $F_\phi = \langle f, \phi_j \rangle_{j=1,\dots,N}$. The jth element of F_ϕ can be expressed as,

$$\int_0^1 f\phi_j dx = \int_{x_{j-1}}^{x_{j+1}} f\phi_j dx = \int_{x_{j-1}}^{x_j} f\phi_j dx + \int_{x_j}^{x_{j+1}} f\phi_j dx.$$

This is justified since anything outside of the range of I_j and I_{j+1} will be zero.
Using the Simpson's rule from (2.18)

$$\int_{x_{j-1}}^{x_j} f\phi_j dx = \frac{h_j}{6}[f(x_{j-1})\phi_j(x_{j-1}) + 4f(x_{j-1/2})\phi_j(x_{j-1/2}) + f(x_j)\phi_j(x_j)].$$

We know that $\phi_j(x_{j-1}) = 0$ and $\phi_j(x_j) = 1$. It can be shown that $\phi_j(x_{j-1/2}) = \phi_j(x_{j+1/2}) = 1/2$. Therefore, the above reduces to

$$\int_{x_{j-1}}^{x_j} f\phi_j dx = \frac{h_j}{6}[2f(x_{j-1/2}) + f(x_j)].$$

Similarly, the integral on(x_j, x_{j+1}) simplifies to

$$\int_{x_j}^{x_{j+1}} f\phi_j dx = \frac{h_{j+1}}{6}[f(x_j) + 2f(x_{j+1/2})].$$

Therefore the integral for the load vector can be given by

$$\begin{aligned}\int_0^1 f\phi_j dx &= \frac{h_j}{6}[2f(x_{j-1/2})+f(x_j)]+\frac{h_j}{6}[f(x_j)+2f(x_{j+1/2})]\\ &= \frac{1}{3}\left[h_j f(x_{j-1/2})+\frac{1}{2}(h_j+h_{j+1})f(x_j)+h_{j+1}f(x_{j+1/2})\right].\end{aligned}$$

If N is large, than we can approximate $f(x_{j-1/2})$ and $f(x_{j+1/2})$ by $f(x_j)$. In this case, we will get,

$$\langle f,\phi_j\rangle = \frac{h_j+h_{j+1}}{2}f(x_j), \quad j=1,\ldots,N. \tag{2.20}$$

For F_ψ, we follow the same procedure to find $\langle f,\psi_j\rangle$,

$$\int_{x_{j-1}}^{x_j} f\psi_j dx = \frac{h_j}{6}[f(x_{j-1})\psi_j(x_{j-1})+4f(x_{j-1/2})\psi_j(x_{j-1/2})+f(x_j)\psi_j(x_j)]. \tag{2.21}$$

We know that $\psi_j(x_{j-1})=0$ and $\psi_j(x_j)=0$. It can be shown that $\phi_j(x_{j-1/2})=-h_j/8$, and $\phi_j(x_{j+1/2})=h_j/8$.

$$\begin{aligned}\psi_j(x_{j-\frac{1}{2}}) &= \frac{1}{h_j^2}\left[x_{j-\frac{1}{2}}^3-(2x_{j-1}+x_j)x_{j-\frac{1}{2}}^2+x_{j-1}(x_{j-1}+2x_j)x_{j-\frac{1}{2}}-x_{j-1}^2x_j\right]\\ &= \frac{1}{h_j^2}\left[\left(x_j-\frac{h_j}{2}\right)^3-(2x_{j-1}+x_j)\left(x_j-\frac{h_j}{2}\right)^2+x_{j-1}(x_{j-1}+2x_j)\left(x_j-\frac{h_j}{2}\right)-x_{j-1}^2x_j\right]\\ &= \frac{1}{h_j^2}\left[\left(x_j-\frac{h_j}{2}\right)^3-(3x_j-2h_j)\left(x_j-\frac{h_j}{2}\right)^2+(x_j-h_j)(3x_j-h_j)\left(x_j-\frac{h_j}{2}\right)-(x_j-h_j)^2x_j\right]\\ &= \frac{1}{h_j^2}\left[-\frac{1}{8}h_j^3\right]\\ &= -\frac{h_j}{8}.\\ \psi_j(x_{j+\frac{1}{2}}) &= \frac{1}{h_j^2}\left[x_{j+\frac{1}{2}}^3-(x_j+2x_{j+1})x_{j+\frac{1}{2}}^2+x_{j+1}(2x_j+x_{j+1})x_{j+\frac{1}{2}}-x_jx_{j+1}^2\right]\\ &= \frac{1}{h_j^2}\left[\left(x_j+\frac{h_j}{2}\right)^3-(x_j+2x_{j+1})\left(x_j+\frac{h_j}{2}\right)^2+x_{j+1}(2x_j+x_{j+1})\left(x_j+\frac{h_j}{2}\right)-x_jx_{j+1}^2\right]\\ &= \frac{1}{h_j^2}\left[\left(x_j+\frac{h_j}{2}\right)^3-(3x_j+2h_j)\left(x_j+\frac{h_j}{2}\right)^2+(x_j+h_j)(3x_j+h_j)\left(x_j+\frac{h_j}{2}\right)-x_j(x_j+h_j)^2\right]\\ &= \frac{1}{h_j^2}\left[\frac{1}{8}h_j^3\right]\\ &= \frac{h_j}{8}.\end{aligned}$$

This integral from (2.21) gets reduced to

$$\int_{x_{j-1}}^{x_j} f\psi_j dx = \frac{h_j}{6}\left[\frac{h_j}{2} f(x_{j-1/2})\right] = \frac{-h_j^2}{12}[f(x_{j-1/2})].$$

Similarly, the integral on (x_j, x_{j+1}) simplifies to

$$\int_{x_j}^{x_{j+1}} f\psi_j dx = \frac{h_{j+1}}{6}\left[\frac{h_j}{2} f(x_{j-1/2})\right] = \frac{h_{j+1}h_j}{12}[f(x_{j+1/2})].$$

Therefore the integral for the load vector can be given by

$$\begin{aligned}\int_0^1 f\psi_j dx &= \frac{-h_j^2}{12}[f(x_{j-1/2})] + \frac{h_{j+1}h_j}{12}[f(x_{j+1/2})] \\ &= \frac{h_j}{12}\left[-h_j f(x_{j-1/2}) + h_{j+1} f(x_{j+1/2})\right].\end{aligned}$$

2.3.2 Stiffness Matrix

For the computation of the stiffness matrix, we will set the interval size I_j, to be the same length. That is, $h_j = h$ for all $j = 1, \cdots, N+1$. This causes the (2.8) and (2.13) to become

$$\phi_j''(x) = \begin{cases} \frac{1}{h^3}\left[-12x + 12x_j - 6h\right] & x \in I_j \\ \frac{1}{h^3}\left[12x - 12x_j - 6h\right] & x \in I_{j+1} \\ 0 & \text{otherwise.} \end{cases} \tag{2.22}$$

and

$$\psi_j''(x) = \begin{cases} \frac{2}{h^2}\left[3x - 3x_j + 2h\right] & x \in I_j \\ \frac{2}{h^2}\left[3x - 3x_j - 2h\right] & x \in I_{j+1} \\ 0 & \text{otherwise.} \end{cases} \tag{2.23}$$

We will be using Simpson's method to approximate the integrals, and therefore it is necessary to compute the values of ϕ_j'' and ψ_j'' at the points $x_{j-1}, x_{j-1/2}, x_j, x_{j+1/2}, x_{j+1}$.

$$\begin{aligned}
\phi_j''(x_{j-1}) &= \frac{6}{h^2}, \qquad \phi_j''(x_{j+1}) = \frac{6}{h^2} \\
\phi_j''(x_{j-1/2}) &= 0, \qquad \phi_j''(x_{j+1/2}) = 0 \\
\phi_j''(x_j) &= -\frac{6}{h^2}, \qquad \psi_j''(x_{j-1}) = -\frac{2}{h}, \qquad (2.24) \\
\psi_j''(x_{j+1}) &= \frac{2}{h}, \qquad \psi_j''(x_{j-1/2}) = \frac{1}{h}, \\
\psi_j''(x_{j+1/2}) &= -\frac{1}{h}, \\
\lim_{x \to x_j^-} \psi_j''(x_j) &= \frac{4}{h}, \\
\lim_{x \to x_j^+} \psi_j''(x_j) &= -\frac{4}{h}. \qquad (2.25)
\end{aligned}$$

We have

$$\begin{aligned}
A_{j,j} &= \left\langle a\phi_j'', \phi_j'' \right\rangle \\
&= \int_{x_{j-1}}^{x_{j+1}} a\left(\phi_j''\right)^2\,dx \\
&= \int_{x_{j-1}}^{x_j} a\left(\phi_j''\right)^2\,dx + \int_{x_j}^{x_{j+1}} a\left(\phi_j''\right)^2\,dx.
\end{aligned}$$

Since

$$\begin{aligned}
\int_{x_{j-1}}^{x_j} a\left(\phi_j''\right)^2\,dx &\approx \frac{h}{6}\left[a_{j-1}\left(\phi_j''(x_{j-1})\right)^2 + 4a_{j-1/2}\left(\phi_j''(x_{j-1/2})\right)^2 + a_j\left(\phi_j''(x_j)\right)^2\right] \\
&= \frac{h}{6}\left[a_{j-1}\frac{36}{h^4} + 4a_{j-1/2}(0) + a_j\frac{36}{h^4}\right] \\
&= \frac{6}{h^3}\left[a_{j-1} + a_j\right] \\
\int_{x_j}^{x_{j+1}} a\left(\phi_j''\right)^2\,dx &\approx \frac{h}{6}\left[a_j\left(\phi_j''(x_j)\right)^2 + 4a_{j+1/2}\left(\phi_j''(x_{j+1/2})\right)^2 + a_{j+1}\left(\phi_j''(x_{j+1})\right)^2\right] \\
&= \frac{h}{6}\left[a_j\frac{36}{h^4} + 4a_{j+1/2}(0) + a_{j+1}\frac{36}{h^4}\right] \\
&= \frac{6}{h^3}\left[a_j + a_{j+1}\right]
\end{aligned}$$

we obtain

$$\begin{aligned} A_{j,j} &= \left\langle a\phi_j'', \phi_j'' \right\rangle \\ &= \int_{x_{j-1}}^{x_{j+1}} a \left(\phi_j''\right)^2 \, dx \\ &= \frac{6}{h^3}\left[a_{j-1} + a_j\right] + \frac{6}{h^3}\left[a_j + a_{j+1}\right] \\ &= \frac{6}{h^3}\left[a_{j-1} + 2a_j + a_{j+1}\right]. \end{aligned}$$

Now for the second diagonal, we have

$$\begin{aligned} A_{j-1,j} &= \left\langle a\phi_j'', \phi_{j-1}'' \right\rangle \\ &= \int_{x_{j-1}}^{x_j} a\phi_j''\phi_{j-1}'' \, dx \\ &\approx \frac{h}{6}\Big[a_{j-1}\phi_j''(x_{j-1})\phi_{j-1}''(x_{j-1}) + 4a_{j-1/2}\phi_j''(x_{j-1/2})\phi_{j-1}''(x_{j-1/2}) + \\ & \quad a_j\phi_j''(x_j)\phi_{j-1}''(x_j)\Big] \\ &= \frac{h}{6}\left[a_{j-1}\frac{-36}{h^4} + 4a_{j-1/2}(0) + a_j\frac{-36}{h^4}\right] \\ &= \frac{-6}{h^3}\left[a_{j-1} + a_j\right]. \end{aligned}$$

We know that the matrix A is symmetric,

$$A_{j,j-1} \approx \frac{-6}{h^3}\left[a_{j-1} + a_j\right].$$

Now using (2.24), we can come up with the entries of matrix C :

$$\begin{aligned} C_{j,j} &= \left\langle a\psi_j'', \psi_j'' \right\rangle \\ &= \int_{x_{j-1}}^{x_{j+1}} a \left(\psi_j''\right)^2 \, dx \\ &= \int_{x_{j-1}}^{x_j} a \left(\psi_j''\right)^2 \, dx + \int_{x_j}^{x_{j+1}} a \left(\psi_j''\right)^2 \, dx. \end{aligned}$$

Since

$$\begin{aligned}
\int_{x_{j-1}}^{x_j} a\left(\psi_j''\right)^2\,dx &\approx \frac{h}{6}\left[a_{j-1}\left(\psi_j''(x_{j-1})\right)^2+4a_{j-1/2}\left(\psi_j''(x_{j-1/2})\right)^2+a_j\left(\psi_j''(x_j)\right)^2\right]\\
&= \frac{h}{6}\left[a_{j-1}\frac{4}{h^2}+4a_{j-1/2}\frac{1}{h^2}+a_j\frac{16}{h^2}\right]\\
&= \frac{2}{3h}\left[a_{j-1}+a_{j-1/2}+4a_j\right]\\
\int_{x_j}^{x_{j+1}} a\left(\psi_j''\right)^2\,dx &\approx \frac{h}{6}\left[a_j\left(\psi_j''(x_j)\right)^2+4a_{j+1/2}\left(\psi_j''(x_{j+1/2})\right)^2+a_{j+1}\left(\psi_j''(x_{j+1})\right)^2\right]\\
&= \frac{h}{6}\left[a_j\frac{16}{h^2}+4a_{j+1/2}\frac{1}{h^2}+a_{j+1}\frac{4}{h^4}\right]\\
&= \frac{2}{3h}\left[4a_j+a_{j+1/2}+a_{j+1}\right]
\end{aligned}$$

we deduce

$$\begin{aligned}
C_{j,j} &= \left\langle a\psi_j'',\psi_j''\right\rangle\\
&\approx \int_{x_{j-1}}^{x_{j+1}} a\left(\psi_j''\right)^2\,dx\\
&= \frac{2}{3h}\left[a_{j-1}+a_{j-1/2}+4a_j\right]+\frac{2}{3h}\left[4a_j+a_{j+1/2}+a_{j+1}\right]\\
&= \frac{2}{3h}\left[a_{j-1}+a_{j-1/2}+8a_j+a_{j+1/2}+a_{j+1}\right].
\end{aligned}$$

Notice that the values of $a_{j-1/2}$ and $a_{j+1/2}$ are not known to me due to the fact that I'm doing this by computational methods. We shall approximate these values,

$$\begin{aligned}
a_{j-1/2} &= \frac{1}{2}(a_{j-1}+a_j),\\
a_{j+1/2} &= \frac{1}{2}(a_j+a_{j+}).
\end{aligned}$$

With these approximations, we shall get

$$\begin{aligned}
C_{j,j} &= \left\langle a\psi_j'',\psi_j''\right\rangle\\
&\approx \frac{2}{3h}\left[a_{j-1}+\frac{1}{2}(a_{j-1}+a_j)+8a_j+\frac{1}{2}(a_j+a_{j+1})+a_{j+1}\right]\\
&\approx \frac{2}{3h}\left[\frac{3}{2}a_{j-1}+9a_j+\frac{3}{2}a_{j+1}\right]\\
&\approx \frac{1}{h}\left[a_{j-1}+6a_j+a_{j+1}\right].
\end{aligned}$$

Now to obtain the second diagonal

$$
\begin{aligned}
C_{j-1,j} &= \langle a\psi_j'', \psi_{j-1}'' \rangle \\
&= \int_{x_{j-1}}^{x_j} a\psi_j'' \psi_{j-1}'' \, dx \\
&\approx \frac{h}{6}[a_{j-1}\psi_j''(x_{j-1})\psi_{j-1}''(x_{j-1}) + 4a_{j-1/2}\psi_j''(x_{j-1/2})\psi_{j-1}''(x_{j-1/2}) + \\
&\quad a_j\psi_j''(x_j)\psi_{j-1}''(x_j)] \\
&= \frac{h}{6}\left[a_{j-1}\frac{8}{h^2} + 4a_{j-1/2}\frac{-1}{h^2} + a_j\frac{8}{h^2}\right] \\
&= \frac{h}{6}\left[a_{j-1}\frac{8}{h^2} + \frac{1}{2}(a_{j-1}+a_j)\frac{-4}{h^2} + a_j\frac{8}{h^2}\right] \\
&= \frac{1}{h}\left[a_{j-1}+a_j\right].
\end{aligned}
$$

We know that the C matrix is symmetric,

$$
C_{j,j-1} \approx \frac{1}{h}\left[a_{j-1}+a_j\right].
$$

Now using the information from (2.24) and (2.25), we can compute the entries of matrix B :

$$
\begin{aligned}
B_{j,j} &= \langle a\psi_j'', \phi_j'' \rangle \\
&= \int_{x_{j-1}}^{x_{j+1}} a\psi_j''\phi_j'' \, dx \\
&= \int_{x_{j-1}}^{x_j} a\psi_j''\phi_j'' \, dx + \int_{x_j}^{x_{j+1}} a\psi_j''\phi_j'' \, dx
\end{aligned}
$$

and we know,

$$
\begin{aligned}
\int_{x_{j-1}}^{x_j} a\psi_j''\phi_j'' \, dx &\approx \frac{h}{6}\left[a_{j-1}\psi_j''(x_{j-1})\phi_j''(x_{j-1}) + 4a_{j-1/2}\psi_j''(x_{j-1/2})\phi_j''(x_{j-1/2}) + a_j\psi_j''(x_j)\phi_j''(x_j)\right] \\
&= \frac{h}{6}\left[a_{j-1}\frac{-12}{h^3} + 4a_{j-1/2}(0) + a_j\frac{-24}{h^3}\right] \\
&= \frac{2}{h^2}\left[-a_{j-1}-2a_j\right].
\end{aligned}
$$

$$
\begin{aligned}
\int_{x_j}^{x_{j+1}} a\psi_j''\phi_j'' \, dx &\approx \frac{h}{6}\left[a_j\psi_j''(x_j)\phi_j''(x_j) + 4a_{j+1/2}\psi_j''(x_{j+1/2})\phi_j''(x_{j+1/2}) + a_{j+1}\psi_j''(x_{j+1})\phi_j''(x_{j+1})\right] \\
&= \frac{h}{6}\left[a_j\frac{24}{h^3} + 4a_{j+1/2}(0) + a_{j+1}\frac{12}{h^3}\right] \\
&= \frac{2}{h^2}\left[2a_j + a_{j+1}\right].
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
B_{j,j} &= \left\langle a\psi_j'', \phi_j'' \right\rangle \\
&\approx \int_{x_{j-1}}^{x_{j+1}} a\psi_j''\phi_j'' dx \\
&= \frac{2}{h^2}\left[-a_{j-1} - 2a_j\right] + \frac{2}{h^2}\left[2a_j + a_{j+1}\right] \\
&= \frac{2}{h^2}\left[-a_{j-1} + a_{j+1}\right] \\
B_{j-1,j} &= \left\langle a\psi_j'', \phi_{j-1}'' \right\rangle \\
&= \int_{x_{j-1}}^{x_j} a\psi_j''\phi_{j-1}''\, dx \\
&\approx \frac{h}{6}\left[a_{j-1}\psi_j''(x_{j-1})\phi_{j-1}''(x_{j-1}) + 4a_{j-1/2}\psi_j''(x_{j-1/2})\phi_{j-1}''(x_{j-1/2}) + a_j\psi_j''(x_j)\phi_{j-1}''(x_j)\right] \\
&= \frac{h}{6}\left[a_{j-1}\frac{12}{h^3} + 4a_{j-1/2}(0) + a_j\frac{24}{h^3}\right] \\
&= \frac{2}{h^2}\left[a_{j-1} + 2a_j\right] \\
B_{j,j-1} &= \left\langle a\psi_{j-1}'', \phi_j'' \right\rangle \\
&= \int_{x_{j-1}}^{x_j} a\psi_{j-1}''\phi_j''\, dx \\
&\approx \frac{h}{6}\left[a_{j-1}\psi_{j-1}''(x_{j-1})\phi_j''(x_{j-1}) + 4a_{j-1/2}\psi_{j-1}''(x_{j-1/2})\phi_j''(x_{j-1/2}) + a_j\psi_{j-1}''(x_j)\phi_j''(x_j)\right] \\
&= \frac{h}{6}\left[a_{j-1}\frac{-24}{h^3} + 4a_{j-1/2}(0) + a_j\frac{-12}{h^3}\right] \\
&= \frac{2}{h^2}\left[-2a_{j-1} - a_j\right].
\end{aligned}
$$

$$
\begin{array}{rcl}
F_{\phi,j} \approx & hf(x_j), & j = 1,\ldots,N \\
F_{\psi,j} \approx & \frac{h^2}{12}[-f(x_{j-1/2}) + f(x_{j+1/2})] & j = 1,\ldots,N \\
A_{j,j} \approx & \frac{6}{h^3}[a_{j-1} + 2a_j + a_{j+1}] & j = 1,\ldots,N \\
A_{j,j-1} = A_{j-1,j} \approx & \frac{-6}{h^3}[a_{j-1} + a_j] & j = 2,\ldots,N \\
B_{j,j} \approx & \frac{2}{h^2}[-a_{j-1} + a_{j+1}] & j = 1,\ldots,N \\
B_{j-1,j} \approx & \frac{2}{h^2}[a_{j-1} + 2a_j] & j = 2,\ldots,N \\
B_{j,j-1} \approx & \frac{-2}{h^2}[2a_{j-1} + a_j] & j = 2,\ldots,N \\
C_{j,j} \approx & \frac{1}{h}[a_{j-1} + 6a_j + a_{j+1}] & j = 1,\ldots,N \\
C_{j,j-1} = C_{j-1,j} \approx & \frac{1}{h}[a_{j-1} + a(x)_j] & j = 2,\ldots,N.
\end{array}
$$

2.4 Numerical Experiments

To demonstrate that the above method works properly, we test it for some examples. There are four examples, in each example we provide the function f, the coefficient $a(x)$, and the compute for the solution u. We also included images comparing the exact solution and the computed solution.

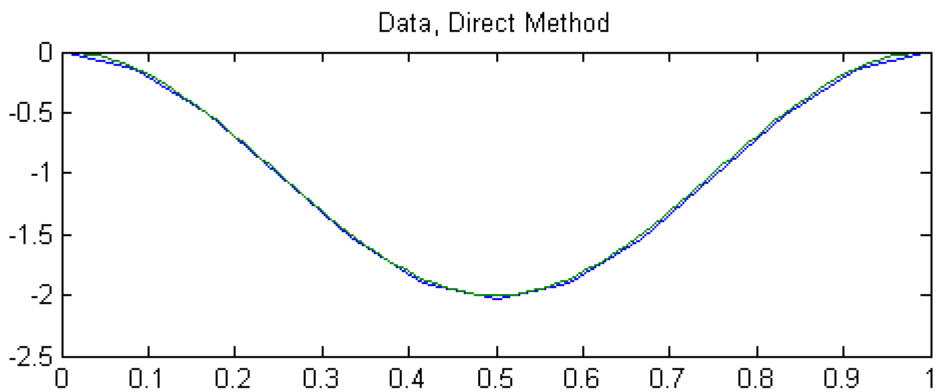


Figure 2.3: Example 1

Example 1:

We have the following data:

$$\begin{aligned} f_1 &= 8\pi^2((2\pi^2(x^2+1)-1)\cos(2\pi x)+4\pi x\sin(2\pi x)) \\ a(x)_1 &= x^2+1 \\ u_1 &= \cos(2\pi x)-1. \end{aligned}$$

Example 2:

We have the following data:

$$\begin{aligned} f_2 &= 4(90x^4-60x^3+42x^2-18x+13) \\ a(x)_2 &= x^4+x^2+2 \\ u_2 &= x^2(x-1)^2. \end{aligned}$$

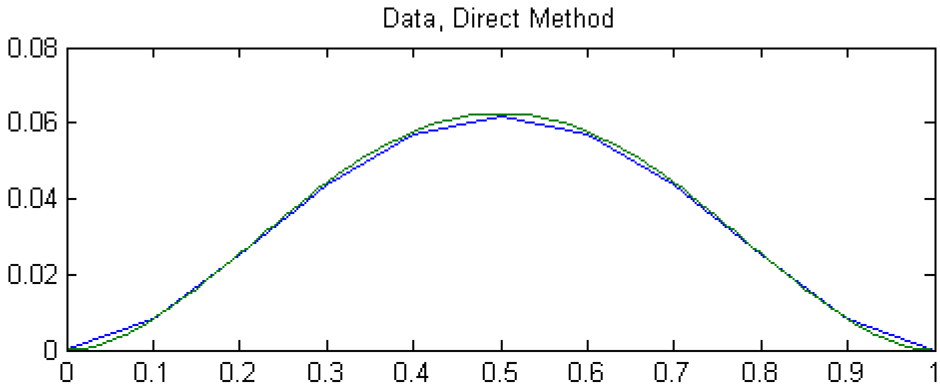


Figure 2.4: Example 2

Example 3:

We have the following data:

$$\begin{aligned}
f_3 &= 32\pi^2(-631.655(x+0.400059)(x^2-1.15006x+0.6095)\cos(4\pi x)-301.593(x-0.25)^2\sin(4\pi x)) \\
a(x)_3 &= (2x-.5)^3+2 \\
u_3 &= \sin(4\pi x-0.5\pi)+1.
\end{aligned}$$

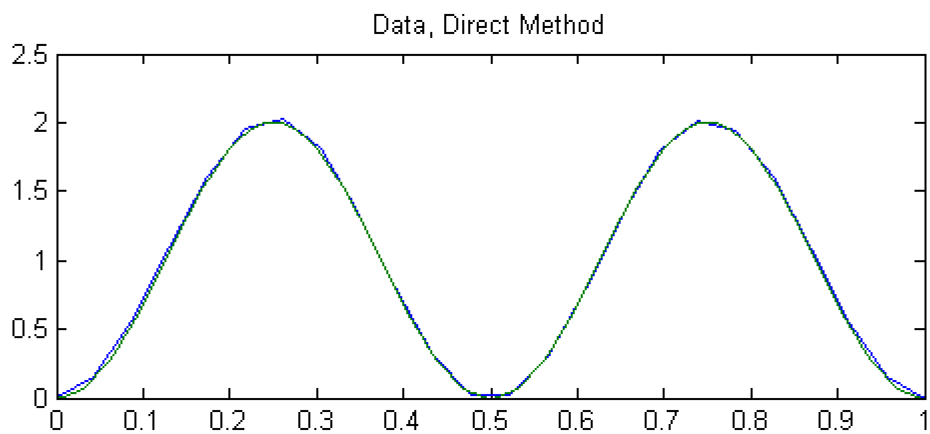


Figure 2.5: Example 3

Example 4:

We have the following data:

$$\begin{aligned} f_4 &= 1764(x-0.773513)(x-0.5)(x-0.226487)(x^2-x+0.687621) \\ a(x)_4 &= (x-0.5)^2+1 \\ u_4 &= x^2(x-1)^2(x-0.5)^3. \end{aligned}$$

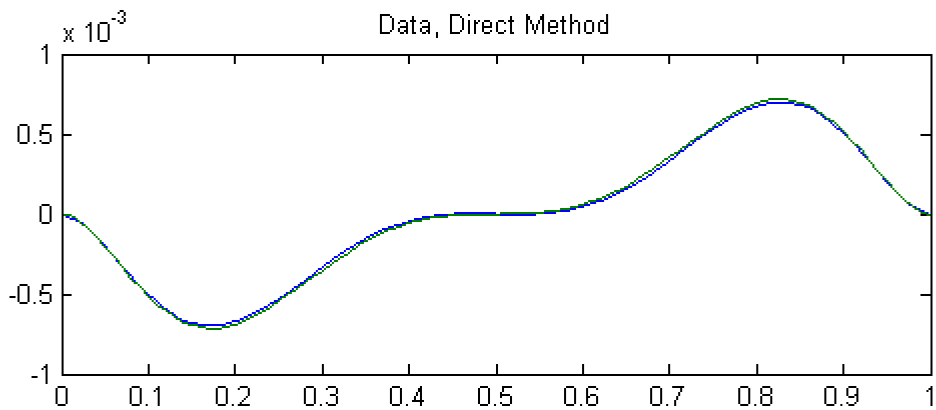


Figure 2.6: Example 4

Chapter 3

Optimization Formulation of Inverse Problems

This chapter investigates the inverse problem as an optimization problem and studies the basic features of the objective functionals. Computable forms of the objective functions are studied in detail.

3.1 Problem Formulation

Recall that we have been dealing with the following static fourth-order boundary value problem in $\Omega = (0,1)$:

$$\begin{aligned} \big(a(x)u''\big)'' &= f(x), 0 < x < 1, & (3.1a)\\ u(0) &= u'(0) = 0, & (3.1b)\\ u(1) &= u'(1) = 0, & (3.1c) \end{aligned}$$

where $a(x)$ is a variable coefficient and f is a suitable function.
The weak form for the above boundary problem reads: Find $u(x) \in V := H_0^2(0,1)$ such that

$$a(u,v) = \langle f,v\rangle \quad \text{for all} \quad v \in V, \tag{3.2}$$

where

$$\begin{aligned} a(u,v) &= \int_0^1 a(x)u''v''\,dx,\\ \langle f,v\rangle &= \int_0^1 f(x)v(x)\,dx. \end{aligned}$$

We assume that the coefficient $a(x)$, in equation (3.2) is strictly positive and constrained between two constants k_0, k_1. That is the set of all admissible coefficients is defined as

$$A := \{a(x)|\ 0 \leq a_0 \leq a(x) \leq a_1\}. \tag{3.3}$$

Since in the analysis the exact role of the coefficient is of vital importance, it is convenient to define a triliear form $T : A \times V \times V \to \mathbb{R}$ by

$$T(a,u,v) = \int_0^1 a(x)u''v''\ dx.$$

The inner product in V is given by:

$$\langle u,v\rangle = \int_0^1 (uv + u'v' + u''v'')\, dx.$$

The corresponding norm is then defined by

$$\|u\|_V^2 = \langle u,v\rangle = \int_0^1 (u^2 + (u')^2 + (u'')^2\, dx.$$

The trilinear form T satisfies the following conditions for all $u, v \in V$, and $a \in \tilde{A}$

$$T(a,u,v) \quad \leq \quad \|a\|_\infty \|u\|_V \|v\|_V \tag{3.4a}$$

$$T(a,u,u) \quad \geq \quad \alpha\|u\|_V^2 \quad \text{where } \alpha > 0 \tag{3.4b}$$

Therefore, we have the variational form: Find $u \in V$ such that

$$T(a,u,v) = m(v) \ \text{ for all } v \in V, \tag{3.5}$$

where

$$m(v) = \int_0^1 f(x)v(x)\ dx.$$

The Lax-Milgram lemma, in view of the above mentioned properties of the trilinear form, ensures that for every $a \in A$, the variation problem (3.5) is uniquely solvable. We can therefore define the coefficient-to-solution map $F : A \to V$ by the condition that $u = F(a)$ is the unique solution of the variational problem.

We recall the following results for the better understanding of the variational form. More details on the following theoretical results can be found in [14] (see also [12], [13], [15], [16], [17] and the cited references therein).

Lemma 3.1.1. *For each $a \in A$, $u = F(a)$ satisfies $\|u\|_V \leq \alpha^{-1}\|m\|_V$.*

Theorem 3.1.1. *The operator F is continuous an*

$$\|F(a)-F(b)\|_V \leq \frac{1}{\alpha}\min\{\|F(a)\|_V\|F(b)\|_V\}\|b-a\|_\infty \text{ for all } a,b\in A. \tag{3.6}$$

Proof. Let $u=F(a)$ and $w=F(b)$, then

$$T(a,u,v)=m(v)=T(b,w,v), \quad \forall v\in V.$$

Substituting $v=u-w$ and manipulating yields

$$T(a,u-w,u-w)=-T(a-b,w,u-w).$$

Then applying conditions (3.4a) and (3.4b), we obtain

$$\alpha\|u-w\|_{\mathrm{V}}^2 \leq \|a-b\|_\infty\|w\|_{\mathrm{V}}\|u-w\|_{\mathrm{V}}$$

and hence

$$\|u-w\|_{\mathrm{V}} \leq \frac{1}{\alpha}\|w\|_{\mathrm{V}}\|a-b\|_\infty = \frac{1}{\alpha}\|F(b)\|_{\mathrm{V}}\|a-b\|_\infty.$$

We can change the roles of a and b, and by bounding $\|F(b)\|_{\mathrm{V}}$ to receive the other minimum bound. □

The following important result discusses the differentiability of $F(a)$.

Theorem 3.1.2. *For each $a\in A$ F is differentiable at a, then $\delta u = DF(a)\delta a$ is an unique solution to the variational equation*

$$T(a,\delta u,v)=-T(\delta a,u,v) \text{ for all } v\in V, \tag{3.7}$$

where $u=F(a)$.

Proof. We know that $u=F(a)$ is the solution of

$$T(a,u,v)=m(v) \text{ for all } v\in V. \tag{3.8}$$

Because of the linearity We can say

$$T(a+\delta a,u+\delta w,v)=m(v) \text{ for all } v\in V \tag{3.9}$$

Now using equations (3.8) and (3.9),

$$\begin{aligned}
T(a,u,v) &= T(a+\delta a,u+\delta w,v)\\
T(a,u,v) &= T(a+\delta a,u,v)+T(a+\delta a,\delta w,v)\\
T(a,u,v) &= T(a,u,v)+T(\delta a,u,v)+T(a+\delta a,\delta w,v).
\end{aligned}$$

Therefore,

$$\begin{aligned}
0 &= -T(a,\delta u,v)+T(a+\delta a,\delta w,v)\\
0 &= -T(a,\delta u,v)+T(a,\delta w,v)+T(\delta a,\delta w,v)\\
0 &= T(a,\delta w-\delta u,v)+T(\delta a,\delta w,v).
\end{aligned}$$

This is true for all $v\in V$, therefore We can choose $v=\delta w-\delta u$ and obtain

$$0=T(a,\delta w-\delta u,\delta w-\delta u)+T(\delta a,\delta w,v).$$

From (3.4), this implies that

$$\begin{aligned}
\alpha\|\delta w-\delta u\|_{\mathrm{V}}^2 &\le T(a,\delta w-\delta u,\delta w-\delta u)\\
T(a,\delta w-\delta u,\delta w-\delta u) &\le \|\delta a\|_\infty\|\delta w\|_{\mathrm{V}}\|\delta w-\delta u\|_{\mathrm{V}}\\
\alpha\|\delta w-\delta u\|_{\mathrm{V}}^2 &\le \|\delta a\|_\infty\|\delta w\|_{\mathrm{V}}\|\delta w-\delta u\|_{\mathrm{V}}\\
\alpha\|\delta w-\delta u\|_{\mathrm{V}} &\le \|\delta a\|_\infty\|\delta w\|_{\mathrm{V}}\\
\|\delta w-\delta u\|_{\mathrm{V}} &\le \frac{1}{\alpha}\|\delta a\|_\infty\|\delta w\|_{\mathrm{V}}. \qquad (3.10)
\end{aligned}$$

This is where We can use the definition of δw and equation (3.6)

$$\begin{aligned}
\|\delta w\|_{\mathrm{V}} &= \|F(a+\delta a)-F(a)\|_{\mathrm{V}}\\
&\le \frac{1}{\alpha}\|F(a\|_{\mathrm{V}}\|(a+\delta a)-a\|_\infty\\
&= \frac{1}{\alpha}\|F(a\|_{\mathrm{V}}\|\delta a\|_\infty.
\end{aligned}$$

We can now use this result with equation (3.10),

$$\begin{aligned}
\|\delta w-\delta u\|_{\mathrm{V}} &\le \frac{1}{\alpha^2}\|F(a)\|_{\mathrm{V}}\|\delta a\|_\infty^2\\
\frac{\|\delta w-\delta u\|_{\mathrm{V}}}{\|\delta a\|_\infty} &\le \frac{1}{\alpha^2}\|F(a)\|_{\mathrm{V}}\|\delta a\|_\infty\\
\frac{\|F(a+\delta a)-F(a)-\delta u\|_{\mathrm{V}}}{\|\delta a\|_\infty} &\le \frac{1}{\alpha^2}\|F(a)\|_{\mathrm{V}}\|\delta a\|_\infty\\
&= \mathbf{O}(\|\delta a\|_\infty).
\end{aligned}$$

Therefore, F is differentiable at a and $DF(a)\delta a=\delta u$ $\square$

3.2 Optimization Formulation: Finite Dimensional Case

We have already discussed the discretized space V_h of the space V. Let A_h be the finite dimensional subspace of B. We consider

$$a \in \mathscr{A} = \{A_h :\ 0 < a_1 \leq a \leq a_2\},$$

which is set of admissible coefficients.
The finite dimensional optimization formulation for the inverse problem of identifying $a(x)$ then takes the form:

$$\min_{a \in \mathscr{A}} J(a) + \varepsilon R(a) \tag{3.11}$$

where $J : A_h \to \mathbb{R}$ and $R : A_h \to \mathbb{R}$ are suitable functionals and $\varepsilon > 0$ a positive parameter. The functional R is the so-called regularization functional and the parameter ε is the so-called regularization parameter.
In the next section, we study the case when the map J is the output least squares functional.

3.3 Output Least-Squares (OLS)

We will now consider the variational problem of (3.7). We first want to choose a to minimize the least output-squares

$$\min_{a \in A} \frac{1}{2} \|u(a) - z\|^2, \tag{3.12}$$

where z is the data and $u(a)$ solves the variational problem

$$\int_0^1 a(x) \left(u''\right) v''\, dx = \int_0^1 f v\, dx \quad \forall v \in V. \tag{3.13}$$

For the finite dimensional analogue of the above functional, we have

$$\begin{aligned} J_1(A) &= \frac{1}{2} \langle u - z, u - z \rangle \\ &= \frac{1}{2} \|u(a) - z, u(a) - z\| \\ &= \frac{1}{2} \int_0^1 (u(a) - z)(u(a) - z) dx \end{aligned}$$

where A is the vector of the nodal values for a.

We have $z \in V_h$ and $u \in V_h$:

$$z = \left[\sum_{i=1}^{n} Z_i \phi_i, \sum_{i=1}^{n} Z_i \psi_i \right]^T$$
$$u = \left[\sum_{i=1}^{n} U_i \phi_i, \sum_{i=1}^{n} U_i \psi_i \right]^T.$$

By letting, $v = u - z$ or $V_i = U_i - Z_i$, we have

$$\begin{aligned}
\|u(a) - z\|^2 &= \langle v, v \rangle \\
&= \left\langle \sum_{i}^{n} V_i \phi_i, \sum_{j}^{n} V_j \phi_j \right\rangle \\
&= \left\langle v_1 \phi_i + \ldots + v_n \phi_n, v_1 \phi_j + \ldots + v_n \phi_n \right\rangle \\
&= V^T A V \\
&= \left\langle \sum_{i}^{n} V_i \psi_i, \sum_{j}^{n} V_j \psi_j \right\rangle \\
&= \left\langle v_1 \psi_i + \ldots + v_n \psi_n, v_1 \psi_j + \ldots + v_n \psi_n \right\rangle \\
&= V^T C V \\
&= \left\langle \sum_{i}^{n} V_i \phi_i, \sum_{j}^{n} V_j \psi_j \right\rangle \\
&= \left\langle v_1 \phi_i + \ldots + v_n \phi_n, v_1 \psi_j + \ldots + v_n \psi_n \right\rangle \\
&= V^T B V \\
&= \left\langle \sum_{i}^{n} V_i \psi_i, \sum_{j}^{n} V_j \phi_j \right\rangle \\
&= \left\langle v_1 \psi_i + \ldots + v_n \psi_n, v_1 \phi_j + \ldots + v_n \phi_n \right\rangle \\
&= V^T B^T V.
\end{aligned}$$

We can put these four submatrices into one cummulative matrix by letting

$$M = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix}.$$

This is the so-called mass matrix.

To summarize:

Entries of $A : A_{ik} = \int_0^1 \phi_i \phi_j \, dx$

Entries of $C: C_{ik} = \int_0^1 \psi_i \psi_j \, dx$
Entries of $B: B_{ik} = \int_0^1 \phi_i \psi_j \, dx.$
To find the mass matrix,

$$
\begin{array}{lclclcl}
A_{i,i} & = & \int_{x_{j-i}}^{x_j} \phi_j^2 dx + \int_{x_j}^{x_{j+1}} \phi_j^2 dx & = & \frac{13}{35}\frac{h^7}{h^6} + \frac{13}{35}\frac{h^7}{h^6} & = & \frac{26}{35}h \\
A_{i-1,i} = a_{i,i-1} & = & \int_{x_{j-i}}^{x_j} \phi_{j-1}\phi_j dx & = & \frac{9}{70}\frac{h^7}{h^6} & = & \frac{9}{70}h \\
B_{i,i} & = & \int_{x_{j-i}}^{x_j} \phi_j \psi_j dx + \int_{x_j}^{x_{j+1}} \phi_j \psi_j dx & = & \frac{11}{210}\frac{h^7}{h^5} - \frac{11}{210}\frac{h^7}{h^5} & = & 0 \\
B_{i-1,i} & = & \int_{x_{j-i}}^{x_j} \phi_j \psi_{j-1} dx & = & \frac{-13}{420}\frac{h^7}{h^5} & = & \frac{-13}{420}h^2 \\
B_{i,i-1} & = & \int_{x_{j-i}}^{x_j} \phi_{j-1} \psi_j dx & = & \frac{13}{420}\frac{h^7}{h^5} & = & \frac{13}{420}h^2 \\
C_{i,i} & = & \int_{x_{j-i}}^{x_j} \psi_j^2 dx + \int_{x_j}^{x_{j+1}} \psi_j^2 dx & = & \frac{1}{105}\frac{h^7}{h^4} + \frac{1}{105}\frac{h^7}{h^4} & = & \frac{2}{105}h^3 \\
C_{i-1,i} = c_{i,i-1} & = & \int_{x_{j-i}}^{x_j} \psi_{j-1}\psi_j dx & = & \frac{-1}{140}\frac{h^7}{h^4} & = & \frac{-1}{140}h^3
\end{array}
$$

We now want to take the gradient of the objective function. We first need to compute

$$\delta V = DF(A)\delta A.$$

From $K(A)V = F$ where $K(A)$ is the stiffness matrix and F is the load vector, we take the derivative with respect to A:

$$
\begin{aligned}
DK(A)\delta AV + K(A)\delta V &= 0 \\
K(A)\delta V &= -DK(\delta A)\delta AV \\
K(A)\delta V &= -K(\delta A)V \\
\delta V &= -K(A)^{-1}DK(\delta A)V
\end{aligned}
$$

We next define the adjoint stiffness matrix $L(V)$ by the condition

$$L(V)A = K(A)V \text{ for all } A \in R^{n+2}, V \in R^n \tag{3.14}$$

We can now say

$$\delta V = -K(A)^{-1}L(V)\delta A. \tag{3.15}$$

We will compute the gradient of J_1

$$
\begin{aligned}
J_1(a) &= \frac{1}{2}(u-z)\cdot M(u-z) \\
DJ_1(a)(\delta a) &= \frac{1}{2}(\delta u-0)\cdot M(u-z)+\frac{1}{2}(u-z)\cdot M(\delta u-0) \\
&= \frac{1}{2}\langle \delta u, M(u-z)\rangle+\frac{1}{2}\langle (u-z), M\delta u\rangle \\
&= \langle \delta u, M(u-z)\rangle \quad \text{where } \delta u=-K(A)^{-1}K(\delta A)V \\
&= -K(A)^{-1}K(\delta A)V \,\cdot\, M(u-z) \\
&= -K(A)^{-1}L(V)\delta A \,\cdot\, M(u-z) \text{ where } L(V)\delta A=K(\delta A)V \\
&= -\delta A \,\cdot\, (K(A)^{-1}L(V))^T M(u-z) \\
&= -\delta A \,\cdot\, L(V)^T K(A)^{-1}M(u-z) \\
\nabla J_0 &= -L(V)^T K(A)^{-1}M(u-z).
\end{aligned}
$$

The adjoint stiffness matrix will be explained more in chapter 4.

3.4 Modified Output Least-Squares (MOLS)

The modified OLS is caused by replacing the L^2 norm by the coefficient-dependent energy norm, and is how we define the objective function, J_2

$$
\begin{aligned}
J_2(A) &= \frac{1}{2}T(a,u(a)-z,u(a)-z) \\
&= \frac{1}{2}(U-Z)K(A)(U-Z).
\end{aligned}
$$

Now to show the gradient of J_2,

$$
\begin{aligned}
J_2(a) &= \frac{1}{2}T(a,u(a)-z,u(a)-z) \\
DJ_2(a)(\delta a) &= \frac{1}{2}T(\delta a,u(a)-z,u(a)-z)+\frac{1}{2}T(a,DU(a)(\delta a,u(a)-z)+\frac{1}{2}T(a,DU(a)(\delta a,u(a)-z) \\
&= \frac{1}{2}T(\delta a,u(a)-z,u(a)-z)+T(a,DU(a)(\delta a,u(a)-z) \\
&= \frac{1}{2}T(\delta a,u(a)-z,u(a)-z)+T(a,\delta u,u(a)-z) \\
&= \frac{1}{2}T(\delta a,u(a)-z,u(a)-z)-T(\delta a,u,u(a)-z) \\
&= \frac{1}{2}T(\delta a,u(a)+z,u(a)-z).
\end{aligned}
$$

For the discrete form:

$$
\begin{aligned}
J_2(A) &= \frac{1}{2}(U-Z)K(A)(U-Z) \\
DJ_2(A)(\delta A) &= \frac{1}{2}\delta\cdot K(A) + \frac{1}{2}(U-Z)\cdot K(A)(\delta U) + \frac{1}{2}(U-Z)\cdot DK(A)(\delta A)(U-Z) \\
&= \delta U\cdot K(A)(U-Z) + \frac{1}{2}(U-Z)\cdot K(\delta A)(U-Z) \\
&= -(K(A)^{-1}L(A)\delta A)\cdot K(A)(U-Z) + \frac{1}{2}(U-Z)\cdot K(\delta A)(U-Z) \\
&= -\delta A\cdot L(U)^T(U-Z) + \frac{1}{2}(U-Z)\cdot K(\delta A)(U-Z) \\
&= -\delta A\cdot L(U)^T(U-Z) + \frac{1}{2}(U-Z)\cdot L(U-Z)\delta A \\
&= -\delta A\cdot L(U)^T(U-Z) + \frac{1}{2}\delta A\cdot L(U-Z)^T(U-Z) \\
&= -\frac{1}{2}\delta A\cdot L(U+Z)^T(U-Z) \\
&= -\frac{1}{2}\delta A\cdot L(U)^T U + \frac{1}{2}\delta A\cdot L(Z)^T Z.
\end{aligned}
$$

Later on in chapter five, We will need the second derivative or the Hessian matrix of the objective functional.

$$
\begin{aligned}
J_2(A) &= \frac{1}{2}(U-Z)K(A)(U-Z) \\
DJ_2(A)(\delta A) &= -\frac{1}{2}\delta A\cdot L(U+Z)^T(U-Z) \\
&= -\frac{1}{2}\delta A\cdot L(U+Z)^T(U-Z) \\
D^2J_2(A)(\delta A,\delta A) &= -\frac{1}{2}\delta A\cdot L(\delta U)^T U - \frac{1}{2}\delta A\cdot L(U)^T\delta U.
\end{aligned}
$$

Take notice that $T_{ijk} = T_{jik}$ so therefore we can say

$$
\begin{aligned}
L(\delta U)^T U &= L(U)^T\delta U \\
\delta U &= K(A)^{-1}L(U)\delta A.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
D^2J_2(A)(\delta A,\delta A) &= -\frac{1}{2}\delta A\cdot L(\delta U)^T U - \frac{1}{2}\delta A\cdot L(U)^T\delta U \\
&= -\delta A\cdot L(U)^T\delta U \\
&= -\delta A\cdot L(U)^T K(A)^{-1}L(U)\delta A.
\end{aligned}
$$

and hence,

$$D^2J_2(A) \;=\; L(U)^T K(A)^{-1} L(U).$$

Summarizing

$$\begin{aligned} J_2(A) &= \frac{1}{2}(U-Z)K(A)(U-Z); \\ DJ_2(A) &= -\frac{1}{2}L(U+Z)^T(U-Z); \\ D^2J_2(A) &= L(U)^T K(A)^{-1} L(U). \end{aligned}$$

3.5 Regularization

From (3.11), we need to minimize a regularization function. The regularization norm can be one of three norms. Each norm represents the Euclidean norm, $\|\cdot\|_2$.

$$\begin{aligned} L_2\text{-norm(square)} \;:\; R_1(a) &= \|a\|^2 \\ &= \int_0^1 a(x)^2 dx \end{aligned}$$

$$\begin{aligned} H_1\text{-norm} \;:\; R_2(a) &: \|a\|^2 + \left\|\frac{da}{dx}\right\|^2 \\ &= \int_0^1 a(x)^2 + \left(\frac{da}{dx}\right)^2 dx \end{aligned}$$

$$\begin{aligned} H_1\text{-semi-norm} \;:\; R_3(a) &= \left\|\frac{da}{dx}\right\|^2 \\ &= \int_0^1 \left(\frac{da}{dx}\right)^2 dx \end{aligned}$$

The discretized regularized norms read:

$$\|a\|^2 = \left\langle \textstyle\sum_{i=0}^{n+1} A_i\phi_j, \sum_{i=0}^{n+1} A_j\phi_j \right\rangle = A^T \bar{M} A$$

$$\left\|\frac{da}{dx}\right\|^2 = \left\langle \textstyle\sum_{i=0}^{n+1} A_i\frac{d\phi_j}{dx}, \sum_{i=0}^{n+1} A_j\frac{d\phi_j}{dx} \right\rangle = A^T \bar{K} A$$

where $\bar{M}$ is a $(N+2)\times(N+2)$ matrix and $\bar{K}$ is a $(N+2)\times(N+2)$ matrix due to not knowing the

boundary values of the coefficient. The regularization term $R(a)$ will be one of three matrices

$$\begin{array}{rcl} L_2\text{-norm(square)} & : & R_1(a) = A^T \bar{M} A \\ H_1\text{-norm} & = & R_2(a) : A^T \bar{M} A + A^T \bar{K} A \\ H_1\text{-simi-norm} & : & R_3(a) = A^T \bar{K} A. \end{array}$$

Throughout this paper we shall use the H_1-norm as the regularization term.

Chapter 4

Identification by Derivative Free Methods

In this chapter we use a derivative free Nelder-Mead method to solve the inverse problem of identifying variable parameters in fourth-order boundary value problem. Derivative free methods are very easy to use as they by pass the stringent requirement of computing the derivatives. However their accuracy is rather limited to small dimension problem.

4.1 Nelder-Mead Method

We have shown that the direct method works, and now we want to show that an iterative derivative free method will work. We chose to use the Nelder-Mead method. This method works by stating with an initial guess of n variables and a radius. Then from the initial guess, $n+1$ vectors are form to creat an n-dimensional simplex. The $n+1$ vertices of this simplex are tested and are arranged in ascending order. The goal is to replace the last value, y_h, this corresponds to the vector $a_h = a_{n+1}$. Then the center of the face of the simplex that omits the a_h vertex is computed, a_c. Then the reflection point is computed, $a_r = a_c - a_h$. If y_r lies in the range of y_1 and y_n, then we replace the worst point, a_h with a_r, and sort the vertices by their functional values and repeat the step.

If y_r is less than y_1, then we expand by setting $a_e = 3a_c - 2a_h$, replace with the better of y_e, or y_r. If y_r is greater than y_n, then we make an outside contraction by setting $a_{oc} = 1.5a_c - 0.5a_h$ or an inside contraction by setting $a_{ic} = 0.5a_c + 0.5a_h$, if the contraction is less then y_h then replace a_h with that value.

If y_h is better than both a_{ic} and a_{oc}, then shrink the simplex by a factor of two in the direction of the minimum a_1, then repeat the steps.

4.2 Nelder-Mead Algorithm

Initialization Step: Choose some radius, and an n-dimensional a^0 initial column vector. Let e be a n-vector size of ones, and e_i be a vector of zeros with a one in the ith position. Let $y_i = J(a_i)$

Step 1: Create vertices

$\sum[(a_0 + \text{radius} * e_i) * e]$

Step 2: Order

$y_1 < y_2 < \cdots < y_{n+1} = yh$

Step 3: Reflection

$a_r = a_c - a_h$

If ($y_1 < y_r < y_n$), then let $a_h = a_r$ go to Step 2.

else if $(y_r < y_1)$, then go to Step 4

else $(y_n < y_r)$, then go to Step 5

Step 4: Expansion

$x_e = 3x_c - 2x_h$

If ($y_e < y_h$), then let $x_h = x_e$ go to step 2.

else $(y_h < y_e)$, then let $x_h = x_r$ go to step 2.

Step 5: Contraction

If $(y_r < y_h)$, then go to 5a.

else $(y_h < y_r)$, then go to 5b.

5a. Outside Contraction

$a_{oc} = 1.5a_c - 0.5a_h$

If ($y_{oc} < y_h$), then let $a_h = a_{oc}$ go to Step 2.

else $(y_h < y_{oc})$, then go to Step 6.

5b. Inside Contraction

$x_{oc} = 0.5a_c + 0.5a_h$

If ($y_{ic} < y_h$), then let $a_h = x_{ic}$ go to Step 2.

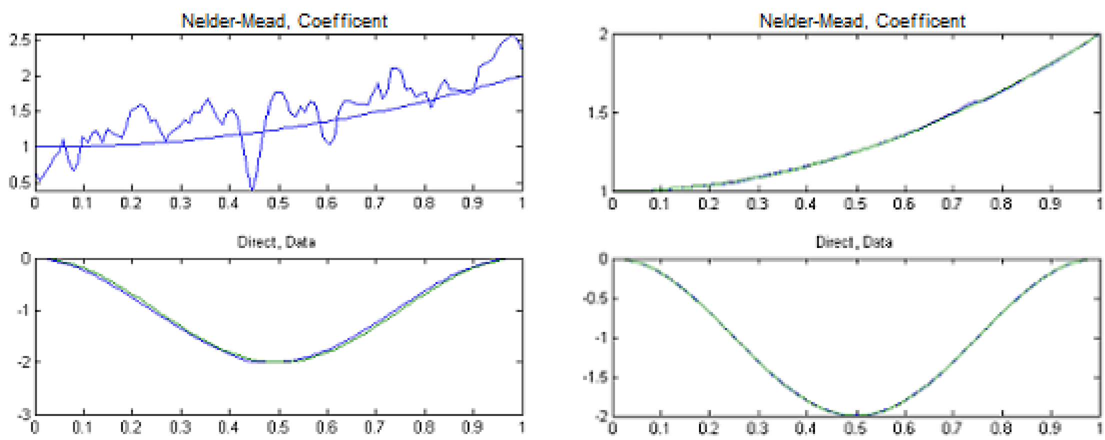
else $(y_h < y_{ic})$, then go to Step 6.

Step 6: Reduction

Shrink

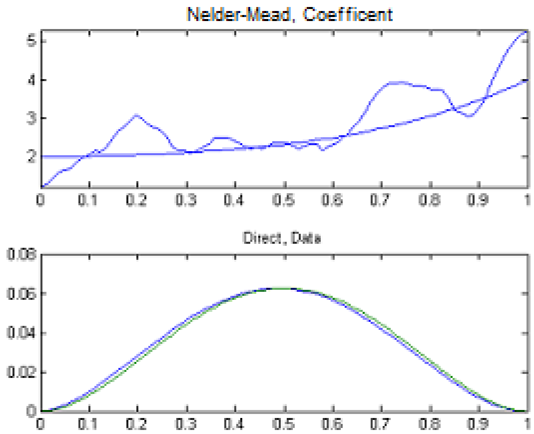
4.3 Numerical Results

In the following results, OLS and MOLS was used along with a regularization norm of H_1-norm. We have used the same four examples that we used for the direct method in Chapter 2. To obtain the optimal regularization parameter ε in the following results, we tested a ranged of values for each example and then picked the one most reliable. The results will show two methods for each result, (a) using OLS, and (b) using MOLS. The top figures in each method will display two lines, the experimented or computed coefficient and the real coefficient. Then the bottom figure is putting the computed coefficient line into (3.2) directly and seeing how closely it matches up to the real data and we'll see it's very close most of the time. In all the cases, the MOLS performs better and converges quickly. Using the iterative Nelder-Mead algorithm for the OLS method took roughly 15 to 30 minutes to run completely, while for the MOLS method for the algorithm took about 2 minutes to complete.

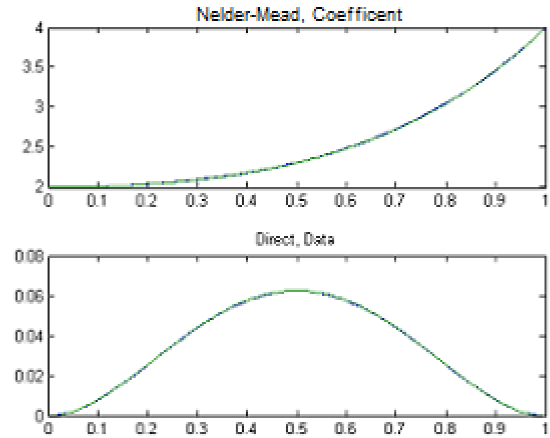


(a) OLS (b) MOLS

Figure 4.1: Example 1 using Nelder-Mead Simplex Method

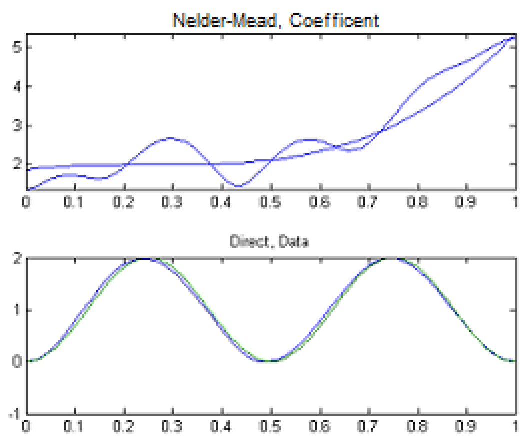


(a) OLS

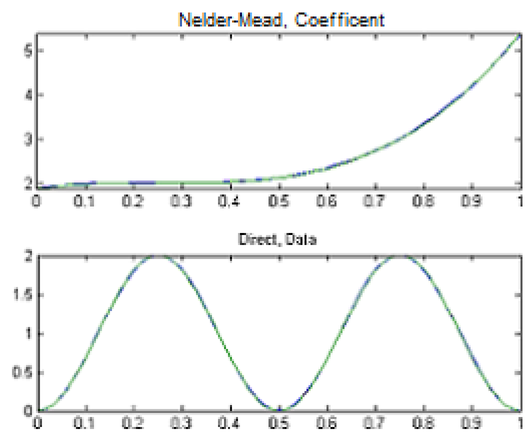


(b) MOLS

Figure 4.2: Example 2 using Nelder-Mead Simplex Method

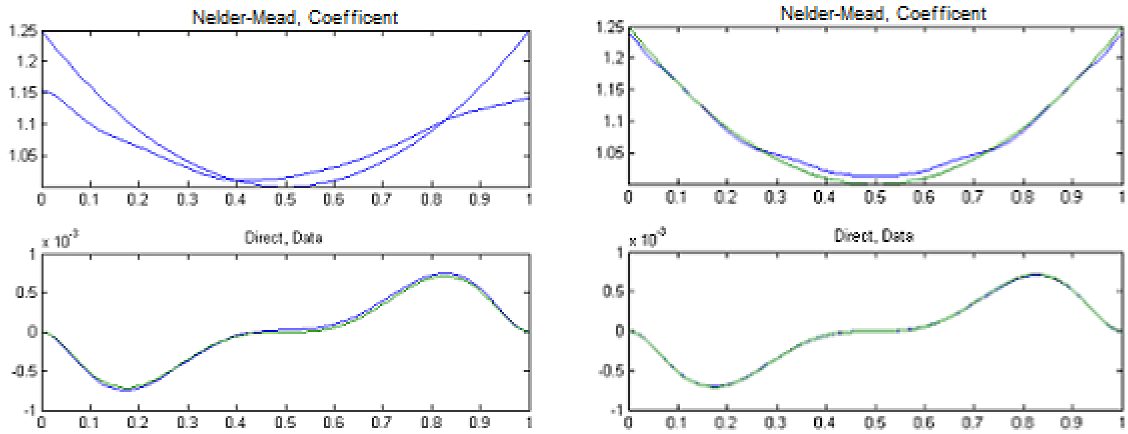


(a) OLS



(b) MOLS

Figure 4.3: Example 3 using Nelder-Mead Simplex Method



(a) OLS (b) MOLS

Figure 4.4: Example 4 using Nelder-Mead Simplex Method

Chapter 5

Computation of the Derivatives

In this chapter we describe the details of the computation of the adjoint stiffness matrix which plays the most fundamental role in the calculation of the derivatives of the objective functionals.

5.1 Adjoint Stiffness Matrix Based Approach

We recall that the adjoint stiffness matrix is defined by the condition

$$L(\tilde{V})\tilde{A} = K(\tilde{A})\tilde{V}, \quad \forall\, \tilde{A} \in \mathbb{R}^{N+2}, \forall\, \tilde{V} \in \mathbb{R}^{2N}, \tag{5.1}$$

where $\tilde{V} = (V, \hat{V})^T$.
Since

$$K(\tilde{A})_{ij} = \int_0^1 a(x)\bar{\phi}_j''\bar{\phi}_i''dx$$

where

$$a(x) = \sum_{k=0}^{n+1} A_k a_k$$

and

$$\bar{\phi} = (\phi, \psi)^T.$$

Therefore, with

$$K(\tilde{A})_{ij} = \sum_{k=0}^{n+1} T_{ijk}\tilde{A}_k$$

where

$$T_{ijk} = \int_0^1 a_k\bar{\phi}_j''\bar{\phi}_i''dx$$

we obtain the formula

$$(K(\tilde{A})\tilde{V})_i = \sum_{j=1}^{n} T_{ijk}\tilde{A}_k\tilde{V}_j.$$

Now using (5.1), we obtain

$$\begin{aligned}
(L(\tilde{V}))_{ik} &= \sum_{j=1}^{2n} T_{ijk}\tilde{V}_j \\
&= \sum_{j=1}^{2n}\left(\int_0^1 a_k\bar{\phi}_j''\bar{\phi}_i''dx\right)V_j \text{ where } \bar{\phi} = \begin{pmatrix}\phi\\ \psi\end{pmatrix} \text{ and} \\
(L(\tilde{V}))_{ik} &= \sum_{j=1}^{n}\left(\int_0^1 a_k\phi_j''\bar{\phi}_i''dx\right)V_j + \sum_{j=1}^{n}\left(\int a_k\psi_j''\bar{\phi}_i''dx\right)\hat{V}_j \\
& \text{where } i = 1,\ldots,2n \text{ and } k = 0,\ldots,n+1.
\end{aligned}$$

Notice that the $L(V)$ matrix has a size of $2n\times(n+2)$, We break the adjoint stiffness matrix L into two blocks of size $n\times(n+2)$ matrices. We will use the notation

$$L = \begin{pmatrix}A+B\\ D+C\end{pmatrix}$$

where

$$\begin{aligned}
A_{ik} &= \sum_{j=1}^{n}\left(\int_0^1 a_k\phi_j''\phi_i''dx\right)V_j \\
B_{ik} &= \sum_{j=1}^{n}\left(\int_0^1 a_k\psi_j''\phi_i''dx\right)\hat{V}_j \\
D_{ik} &= \sum_{j=1}^{n}\left(\int_0^1 a_k\phi_j''\psi_i''dx\right)V_j \\
C_{ik} &= \sum_{j=1}^{n}\left(\int_0^1 a_k\psi_j''\psi_i''dx\right)\hat{V}_j.
\end{aligned}$$

The basis functions for ϕ and ψ are as defined in Chapter 2.

Also from Chapter 2, we need the second derivatives at different x-values which are:

$$\begin{aligned}
\phi_j''(x_{j-1}) &= \phi_j''(x_{j+1}) = \frac{6}{h^2} \\
\phi_j''(x_{j-1/2}) &= \phi_j''(x_{j+1/2}) = 0 \\
\phi_j''(x_j) &= -\frac{6}{h^2}
\end{aligned}$$

$$\begin{array}{rr}
\psi_j''(x_{j-1}) = -\dfrac{2}{h} & \psi_j''(x_{j-1/2}) = \dfrac{1}{h} \\
\psi_j''(x_{j+1/2}) = -\dfrac{1}{h} & \psi_j''(x_{j+1}) = \dfrac{2}{h} \\
\lim\limits_{x \to x_{j-}} \psi_j''(x) = \dfrac{4}{h} & \lim\limits_{x \to x_{j+}} \psi_j''(x) = -\dfrac{4}{h}.
\end{array}$$

We will denote I_i to be the i-th subinterval $[x_{i-1}, x_i]$. It is important to note that support of both ϕ_i and ψ_i is $I_i \cup I_{i+1}$.

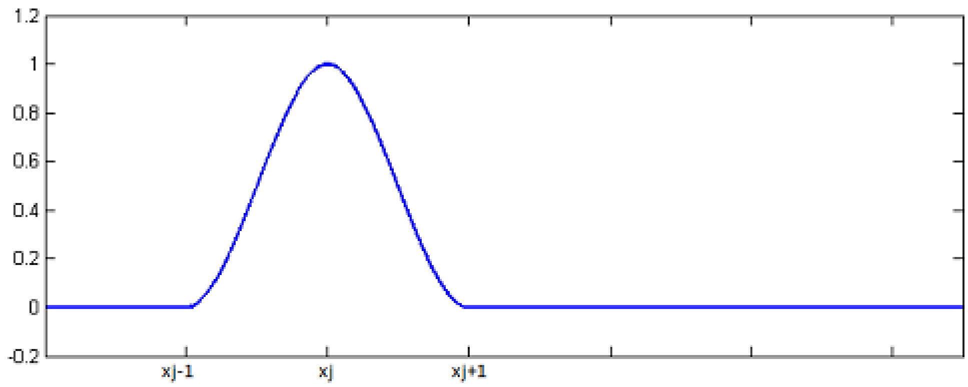


Figure 5.1: Basis function ϕ_j

We first construct the matrix A.

$$A_{ik} = \sum_{j=1}^{n} \left(\int a_k \phi_j'' \phi_i'' dx \right) V_j \text{ for } i = 1, .., n \text{ and } k = 0, ...n+1.$$

We start with the first row ($i = 1$) and the index k varies from 0 to $n+1$. When $k = 0$, notice that the basis function for w_0 has non-zero values only on I_1.

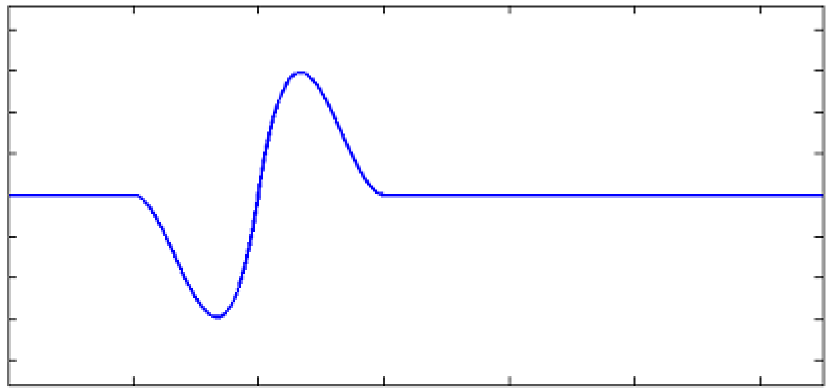


Figure 5.2: Basis function ψ_j

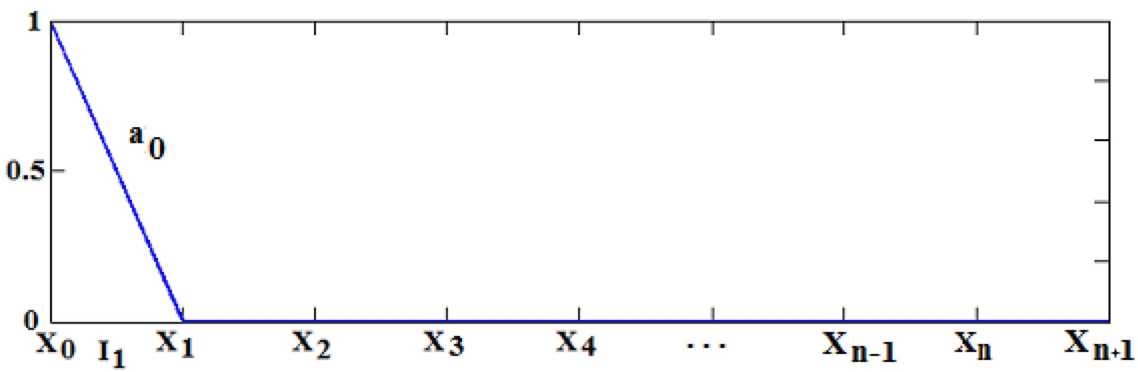


Figure 5.3: Basis function a_0

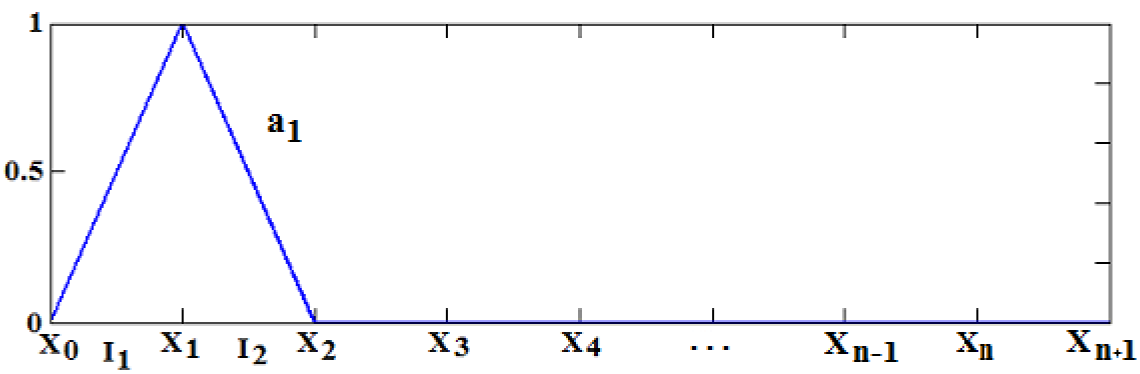


Figure 5.4: Basis function a_1

We have

$$
\begin{aligned}
A_{10} &= \sum_{j=1}^{n}\left(\int_0^1 a_0\phi_j''\phi_1''dx\right)V_j \\
&= V_1\int_0^1 a_0\left(\phi_1''\right)^2 dx \\
&= V_1\int_{I_1} a_0\left(\phi_1''\right)^2 dx \\
&= V_1\frac{h/2}{3}\left[a_0(x_0)\left(\phi_1''(x_0)\right)^2+4a_0(x_{1/2})\left(\phi_1''(x_{1/2})\right)^2+a_0(x_1)\left(\phi_j''(x_1)\right)^2\right] \\
&= V_1\frac{h}{6}\left[1\cdot\left(\frac{6}{h^2}\right)^2+4\cdot\frac{1}{2}\cdot 0+0\cdot\left(-\frac{6}{h^2}\right)^2\right] \\
&= \frac{6}{h^3}V_1.
\end{aligned}
$$

where we used Simpson's Rule for the integration. For $k=1$ we notice that the basis function a_1 has non-zero values only on I_1 and I_2. We are collecting all nonzero terms involving basis functions ϕ_1 and ϕ_2. Then

$$
\begin{aligned}
A_{11} &= \sum_{j=1}^{n}\left(\int_0^1 a_1\phi_j''\phi_1''dx\right)V_j \\
&= V_1\int_0^1 a_1\left(\phi_1''\right)^2 dx+V_2\int a_1\phi_2''\phi_1''dx \\
&= V_1\int_{I_1} a_1\left(\phi_1''\right)^2 dx+V_1\int_{I_2} a_1(\phi_1'')^2 dx+V_2\int_{I_2} a_1\phi_2''\phi_1''dx \\
&= V_1\frac{h}{6}\left[a_1(x_0)\left(\phi_1''(x_0)\right)^2+4a_1(x_{1/2})\left(\phi_1''(x_{1/2})\right)^2+a_1(x_1)\left(\phi_1''(x_1)\right)^2\right] \\
&\quad +V_1\frac{h}{6}\left[a_1(x_1)\left(\phi_1''(x_1)\right)^2+4a_1(x_{3/2})\left(\phi_1''(x_{3/2})\right)^2+a_1(x_2)\left(\phi_1''(x_2)\right)^2\right] \\
&\quad +V_2\frac{h}{6}\left[a_1(x_1)\phi_2''(x_1)\phi_1''(x_1)+4a_1(x_{3/2})\phi_2''(x_{3/2})\phi_1''(x_{3/2})+a_1(x_2)\phi_2''(x_2)\phi_1''(x_2)\right] \\
&= V_1\frac{h}{6}\left(-\frac{6}{h^2}\right)^2+V_1\frac{h}{6}\left(-\frac{6}{h^2}\right)^2+V_2\frac{h}{6}\left(\frac{6}{h^2}\right)\left(-\frac{6}{h^2}\right) \\
&= \frac{6}{h^3}(2V_1-V_2).
\end{aligned}
$$

When $k=2$, we notice that the basis function a_2 has non-zero values only on I_2 and I_3. Similarly,

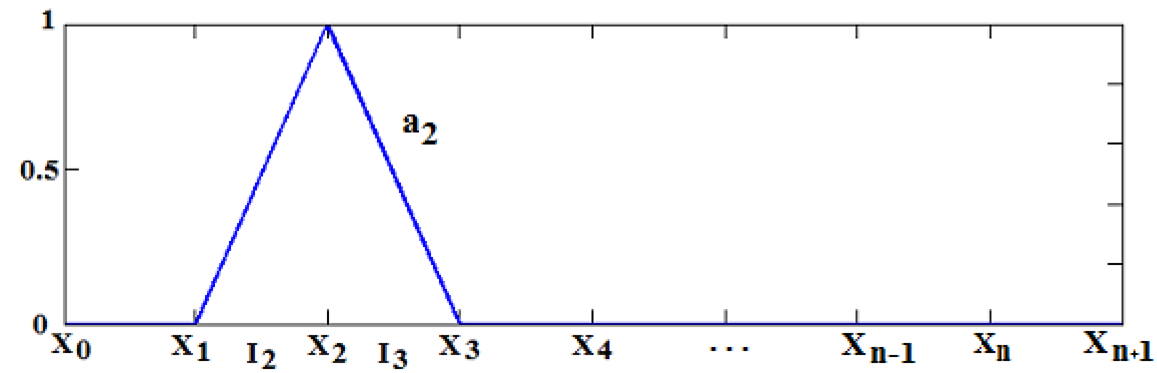


Figure 5.5: Basis function a_2

$$
\begin{aligned}
A_{12} &= \sum_{j=1}^{n}\left(\int_0^1 a_2\phi_j''\phi_1''dx\right)V_j \\
&= V_1\int_0^1 a_2\left(\phi_1''\right)^2dx + V_2\int a_2\phi_2''\phi_1''dx \\
&= V_1\int_{I_2} a_2\left(\phi_1''\right)^2dx + V_2\int_{I_2} a_2\phi_2''\phi_1''dx \\
&= V_1\frac{h}{6}\left[a_2(x_1)\left(\phi_1''(x_1)\right)^2 + 4a_2(x_{3/2})\left(\psi_1''(x_{3/2})\right)^2 + a_2(x_2)\left(\phi_1''(x_2)\right)^2\right] \\
&\quad + V_2\frac{h}{6}\left[a_2(x_1)\phi_2''(x_1)\phi_1''(x_1) + 4a_2(x_{3/2})\phi_2''(x_{3/2})\phi_1''(x_{3/2}) + a_2(x_2)\phi_2''(x_2)\phi_1''(x_2)\right] \\
&= V_1\frac{h}{6}\left(\frac{6}{h^2}\right)^2 + V_2\frac{h}{6}\left(-\frac{6}{h^2}\right)\left(\frac{6}{h^2}\right) \\
&= \frac{6}{h^3}(V_1 - V_2).
\end{aligned}
$$

When $k=3$, we notice that the basis function a_3 has non-zero values only on I_3 and I_4, and these subintervals have no overlapping with the support of ϕ_k if $k \geq 3$. Therefore $A_{1k}=0$ for $k \geq 3$.

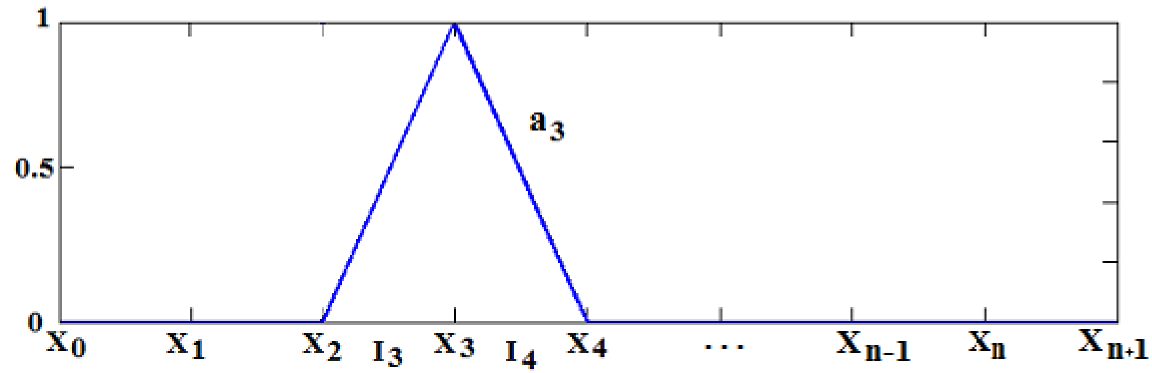


Figure 5.6: Basis function a_3

For the second row of matrix A we have

$$
\begin{aligned}
A_{20} &= 0 \\
A_{21} &= \sum_{j=1}^{n} \left(\int_0^1 a_1 \phi_j'' \phi_2'' dx \right) V_j \\
&= V_1 \int_0^1 a_1 \phi_1'' \phi_2'' dx + V_2 \int_0^1 a_1 \left(\phi_2''\right)^2 dx \\
&= V_1 \int_{I_2} a_2 \phi_1'' \phi_2'' dx + V_2 \int_{I_2} a_2 \left(\phi_2''\right)^2 dx \\
&= V_1 \frac{h}{6} \left[a_2(x_1)\phi_1''(x_1)\phi_2''(x_1) + 4a_2(x_{3/2})\phi_1''(x_{3/2})\phi_2''(x_{3/2}) + a_2(x_2)\phi_1''(x_2)\phi_2''(x_2) \right] \\
&\quad + V_2 \frac{h}{6} \left[a_2(x_1)(\phi_2''(x_1))^2 + 4a_2(x_{3/2})(\phi_2''(x_{3/2}))^2 + a_2(x_2)(\phi_2''(x_2))^2 \right] \\
&= V_1 \frac{h}{6} \left(\frac{6}{h^2} \right) \left(-\frac{6}{h^2} \right) + V_2 \frac{h}{6} \left(-\frac{6}{h^2} \right)^2 \\
&= \frac{6}{h^3}(-V_1 + V_2).
\end{aligned}
$$

$$
\begin{aligned}
A_{22} &= \sum_{j=1}^{n}\left(\int_0^1 a_2\phi_j''\phi_2''dx\right)V_j \\
&= V_1\int_0^1 a_2\phi_1''\phi_2''dx + V_2\int_0^1 a_2\left(\phi_2''\right)^2dx + V_3\int a_2\phi_3''\phi_2''dx \\
&= V_1\int_{I_2} a_2\phi_1''\phi_2''dx + V_2\int_{I_2} a_2\left(\phi_2''\right)^2dx + V_2\int_{I_3} a_2\left(\phi_2''\right)^2dx + V_3\int_{I_3} a_2\phi_1''\phi_2''dx \\
&= V_1\frac{h}{6}\left[a_2(x_1)\phi_1''(x_1)\phi_2''(x_1) + 4a_1(x_{3/2})\phi_1''(x_{3/2})\phi_2''(x_{3/2}) + a_2(x_2)\phi_1''(x_2)\phi_2''(x_2)\right] \\
&\quad +V_1\frac{h}{6}\left[a_2(x_1)\left(\phi_2''(x_1)\right)^2 + 4a_1(x_{3/2})\left(\phi_2''(x_{3/2})\right)^2 + a_2(x_2)\left(\phi_2''(x_2)\right)^2\right] \\
&\quad +V_2\frac{h}{6}\left[a_2(x_2)\left(\phi_2''(x_2)\right)^2 + 4a_1(x_{5/2})\left(\phi_2''(x_{5/2})\right)^2 + a_2(x_3)\left(\phi_2''(x_3)\right)^2\right] \\
&\quad +V_3\frac{h}{6}\left[a_2(x_2)\phi_3''(x_2)\phi_2''(x_2) + 4a_2(x_{5/2})\phi_3''(x_{5/2})\phi_2''(x_{5/2}) + a_2(x_3)\phi_3''(x_3)\phi_2''(x_3)\right] \\
&= V_1\frac{h}{6}\left(\frac{6}{h^2}\right)\left(-\frac{6}{h^2}\right) + V_1\frac{h}{6}\left(-\frac{6}{h^2}\right)^2 + V_2\frac{h}{6}\left(-\frac{6}{h^2}\right)^2 + V_3\frac{h}{6}\left(\frac{6}{h^2}\right)\left(-\frac{6}{h^2}\right) \\
&= \frac{6}{h^3}(-V_1 + 2V_2 - V_3).
\end{aligned}
$$

$$
\begin{aligned}
A_{23} &= \sum_{j=1}^{n}\left(\int_0^1 a_3\phi_j''\phi_2''dx\right)V_j \\
&= V_2\int_0^1 a_3\left(\phi_2''\right)^2dx + V_3\int_0^1 a_3\phi_3''\phi_2''dx \\
&= V_2\int_{I_3} a_3\left(\phi_2''\right)^2dx + V_2\int_{I_3} a_3\phi_3''\phi_2''dx \\
&= V_2\frac{h}{6}\left[a_3(x_2)\left(\phi_2''(x_2)\right)^2 + 4a_3(x_{5/2})\left(\phi_2''(x_{5/2})\right)^2 + a_3(x_3)\left(\phi_2''(x_3)\right)^2\right] \\
&\quad +V_3\frac{h}{6}\left[a_3(x_2)\phi_3''(x_2)\phi_2''(x_2) + 4a_3(x_{5/2})\phi_3''(x_{5/2})\phi_2''(x_{5/2}) + a_3(x_3)\phi_3''(x_3)\phi_2''(x_3)\right] \\
&= V_2\frac{h}{6}\left(\frac{6}{h^2}\right)^2 + V_3\frac{h}{6}\left(-\frac{6}{h^2}\right)\left(\frac{6}{h^2}\right) \\
&= \frac{6}{h^3}(V_2 - V_3).
\end{aligned}
$$

Notice that

$$A_{2k} = 0 \text{ for } k \geq 4.$$

This pattern will continue up to the row $N-1$,

$$\begin{aligned}
A_{n-1,k} &= 0 \text{ for } k \leq n-3 \\
A_{n-1,n-2} &= \frac{6}{h^3}(-V_{n-2}+V_{n-1}) \\
A_{n-1,n-1} &= \frac{6}{h^3}(-V_{n-2}+2V_{n-1}-V_n) \\
A_{n-1,n} &= \frac{6}{h^3}(V_{n-1}-V_n) \\
A_{n-1,n+1} &= 0.
\end{aligned}$$

For the last row, the n-th,

$$A_{n,k} = 0 \text{ for } k \leq n-2.$$

When $k = n-1$ the basis function a_{n-1} will have non-zero values only on of I_{n-1} and I_n, so

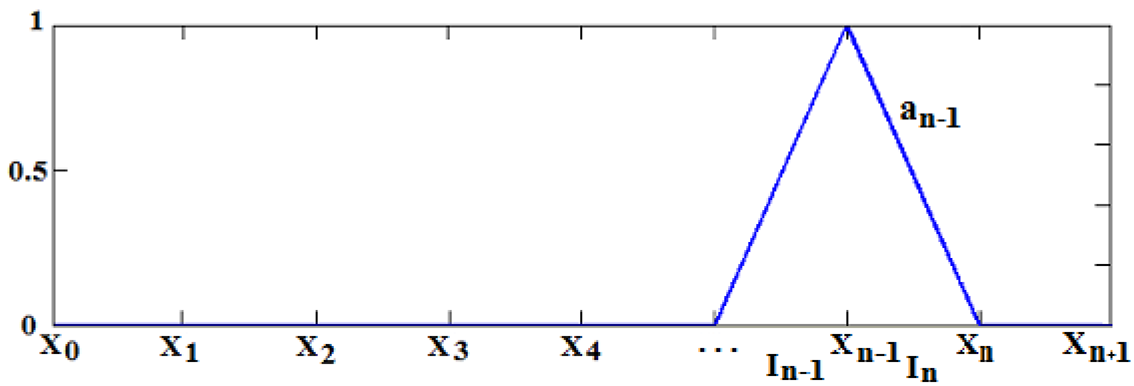


Figure 5.7: Basis function a_{n-1}

$$\begin{aligned}
A_{n,n-1} &= \sum_{j=1}^{n}\left(\int_0^1 a_{n-1}\phi_j''\phi_n'' dx\right)V_j \\
&= V_{n-1}\int_{I_n} a_{n-1}\phi_{n-1}\phi_n'' dx + V_n\int_{I_n} a_{n-1}\left(\phi_n''\right)^2 dx \\
&= V_{n-1}\frac{h}{6}\left[a_{n-1}(x_{n-1})\phi_{n-1}''(x_{n-1})\phi_n''(x_{n-1}) + 4a_{n-1}(x_{n-1/2})\phi_{n-1}''(x_{n-1/2})\phi_n''(x_{n-1/2})\right. \\
&\quad \left. + a_{n-1}(x_n)\phi_{n-1}''(x_n)\phi_n''(x_n)\right] + V_n\frac{h}{6}\left[a_{n-1}(x_{n-1})\left(\phi_n''(x_{n-1})\right)^2\right. \\
&\quad \left. + 4a_{n-1}(x_{n-1/2})\left(\phi_n''(x_{n-1/2})\right)^2 + a_{n-1}(x_n)\left(\phi_n''(x_n)\right)^2\right] \\
&= V_{n-1}\frac{h}{6}\left[\left(-\frac{6}{h^2}\right)\left(\frac{6}{h^2}\right)\right] + V_n\frac{h}{6}\left[\left(\frac{6}{h^2}\right)^2\right] \\
&= \frac{6}{h^3}(-V_{n-1}+V_n).
\end{aligned}$$

When $k=n$, notice that the basis function a_n has non-zero values only on I_n and I_{n+1}.

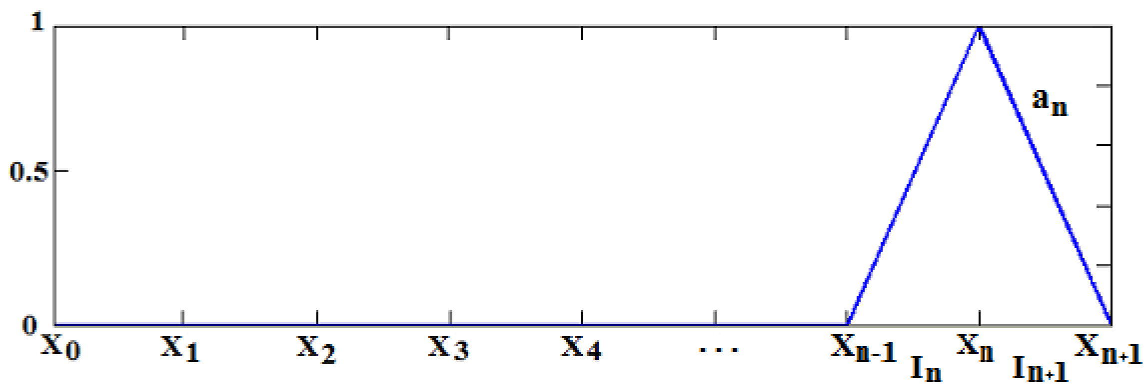


Figure 5.8: Basis function a_n

Then

$$\begin{aligned}
A_{n,n} &= \sum_{j=1}^{n}\left(\int_0^1 a_n\phi_j''\phi_n'' dx\right)V_j \\
&= V_{n-1}\int_{I_n} a_n\phi_{n-1}''\phi_n'' dx + V_n\int_{I_n} a_n(\phi_n'')^2 dx + V_n\int_{I_{n+1}} a_n(\phi_n'')^2 dx \\
&= V_{n-1}\frac{h}{6}\left[\left(\frac{6}{h^2}\right)\left(-\frac{6}{h^2}\right)\right] + V_n\frac{h}{6}\left[\left(-\frac{6}{h^2}\right)^2\right] + V_n\frac{h}{6}\left[\left(-\frac{6}{h^2}\right)^2\right] \\
&= \frac{6}{h^3}(-V_{n-1}+2V_n).
\end{aligned}$$

For $k = n+1$ the basis function a_{n+1} has non-zero values only on I_{n+1}.

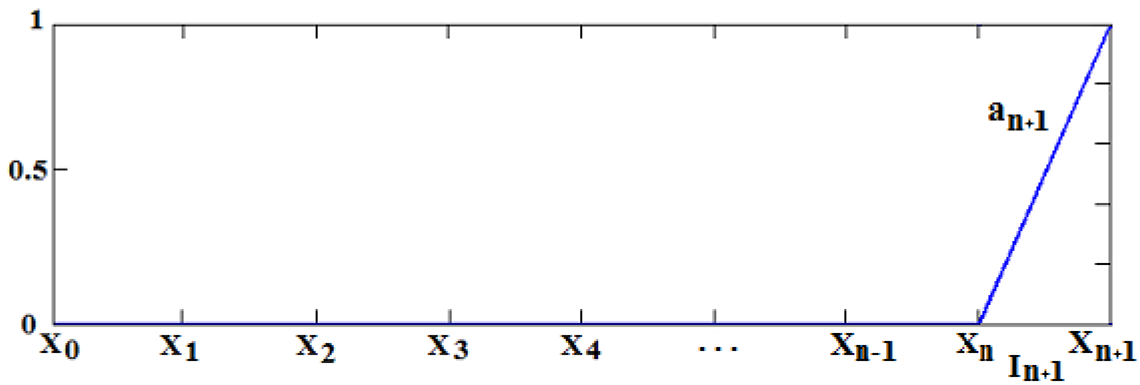


Figure 5.9: Basis functions a_{n+1}

Therefore

$$\begin{aligned}
A_{n,n+1} &= \sum_{j=1}^{n}\left(\int_0^1 a_{n+1}\phi_j''\phi_n''dx\right)V_j = V_n\int_{I_{n+1}} a_{n+1}\left(\phi_n''\right)^2 dx\\
&= V_n\frac{h}{6}\left[a_{n+1}(x_n)\left(\phi_n''(x_n)\right)^2 + 4a_{n+1}(x_{n+1/2})\left(\phi_n''(x_{n+1/2})\right)^2 + a_{n+1}(x_{n+1})\left(\phi_n''(x_{n+1})\right)^2\right]\\
&= V_n\frac{h}{6}\left[\left(\frac{6}{h^2}\right)^2\right]\\
&= \frac{6}{h^3}V_n.
\end{aligned}$$

Putting together the entries of we get the following matrix:

$$A = \frac{6}{h^3}\begin{pmatrix}
V_1 & 2V_1 - V_2 & V_1 - V_2 & 0 & 0 & \dots & 0\\
0 & -V_1 + V_2 & -V_1 + 2V_2 - V_3 & V_2 - V_3 & 0 & \dots & 0\\
0 & \dots & -V_2 + V_3 & -V_2 + 2V_3 - V_4 & V_3 - V_4 & \dots & 0\\
 & & & \vdots & & & \\
0 & \dots & 0 & -V_{\text{n-2}} + V_{\text{n-1}} & -V_{\text{n-2}} + 2V_{\text{n-1}} - V_n & V_{\text{n-1}} - V_n & 0\\
0 & \dots & 0 & 0 & -V_{\text{n-1}} + V_n & -V_{\text{n-1}} + 2V_n & V_n
\end{pmatrix}.$$

We evaluate the entires of matrix B in a similar manner. Recall that the entries of matrix B are defined by

$$B_{ik} = \sum_{j=1}^{n}\left(\int a_k\psi_j''\phi_i''dx\right)\hat{V}_j \text{ for } i = 1,..,n \text{ and } k = 0,...n+1.$$

We start with the first row.

$$
\begin{aligned}
B_{10} &= \sum_{j=1}^{n}\left(\int_0^1 a_0\psi_j''\phi_1''dx\right)\hat{V}_j\\
&= \hat{V}_1\int_0^1 a_0\psi_1''\phi_1''dx\\
&= \hat{V}_1\frac{h/2}{3}\left[a_0(x_0)\psi_1''(x_0)\phi_1''(x_0)+4a_0(x_{1/2})\psi_1''(x_{1/2})\phi_1''(x_{1/2})+a_0(x_1)\psi_1''(x_1)\phi_1''(x_1)\right]\\
&= \hat{V}_1\frac{h}{6}\left[\left(-\frac{2}{h}\right)\left(\frac{6}{h^2}\right)+0+0\right]\\
&= -\frac{2}{h^2}\hat{V}_1.
\end{aligned}
$$

$$
\begin{aligned}
B_{11} &= \sum_{j=1}^{n}\left(\int_0^1 a_1\psi_j''\phi_1''dx\right)\hat{V}_j\\
&= \hat{V}_1\int_0^1 a_1\psi_1''\phi_1''dx+\hat{V}_2\int_0^1 a_1\psi_2''\phi_1''dx\\
&= \hat{V}_1\int_{I_1} a_1\psi_1''\phi_1''dx+\hat{V}_1\int_{I_2} a_1\psi_1''\phi_1''dx+\hat{V}_2\int_{I_2} a_1\psi_2''\phi_1''dx\\
&= \hat{V}_1\frac{h}{6}\left[a_1(x_0)\psi_1''(x_0)\phi_1''(x_0)+4a_1(x_{1/2})\psi_1''(x_{1/2})\phi_1''(x_{1/2})+a_1(x_1)\psi_1''(x_1)\phi_1''(x_1)\right]+\\
&\quad \hat{V}_1\frac{h}{6}\left[a_1(x_1)\psi_1''(x_1)\phi_1''(x_1)+4a_1(x_{3/2})\psi_1''(x_{3/2})\phi_1''(x_{3/2})+a_1(x_2)\psi_1''(x_2)\phi_1''(x_2)\right]+\\
&\quad \hat{V}_2\frac{h}{6}\left[a_1(x_1)\psi_2''(x_1)\phi_1''(x_1)+4a_1(x_{3/2})\psi_2''(x_{3/2})\phi_1''(x_{3/2})+a_1(x_2)\psi_2''(x_2)\phi_1''(x_2)\right]\\
&= \hat{V}_1\frac{h}{6}\left(\frac{4}{h}\right)\left(-\frac{6}{h^2}\right)+\hat{V}_1\frac{h}{6}\left(-\frac{4}{h}\right)\left(-\frac{6}{h^2}\right)+\hat{V}_2\frac{h}{6}\left(-\frac{2}{h}\right)\left(-\frac{6}{h^2}\right)\\
&= \frac{2}{h^2}\hat{V}_2.
\end{aligned}
$$

$$
\begin{aligned}
B_{12} &= \sum_{j=1}^{n}\left(\int_0^1 a_2\psi_j''\psi_1''dx\right)\hat{V}_j \\
&= \hat{V}_1\int_0^1 a_2\psi_1''\phi_1''dx + \hat{V}_2\int_0^1 a_2\psi_2''\phi_1''dx \\
&= \hat{V}_1\int_{I_2} a_2\psi_1''\phi_1''dx + \hat{V}_2\int_{I_2} a_2\psi_2''\phi_1''dx \\
&= \hat{V}_1\frac{h}{6}\left[a_2(x_1)\psi_1''(x_1)\phi_1''(x_1) + 4a_2(x_{3/2})\psi_1''(x_{3/2})\phi_1''(x_{3/2}) + a_2(x_2)\psi_1''(x_2)\phi_1''(x_2)\right] + \\
&\quad \hat{V}_2\frac{h}{6}\left[a_2(x_1)\psi_2''(x_1)\phi_1''(x_1) + 4a_2(x_{3/2})\psi_2''(x_{3/2})\phi_1''(x_{3/2}) + a_2(x_2)\psi_2''(x_2)\phi_1''(x_2)\right] \\
&= \hat{V}_1\frac{h}{6}\left(\frac{2}{h}\right)\left(\frac{6}{h^2}\right) + \hat{V}_2\frac{h}{6}\left(\frac{4}{h}\right)\left(\frac{6}{h^2}\right) \\
&= \frac{2}{h^2}\left(\hat{V}_1 + 2\hat{V}_2\right). \\
B_{1k} &= 0 \quad \text{for } k \geq 3.
\end{aligned}
$$

Now let's look at the 2nd row. We have

$$B_{20} = 0.$$

$$
\begin{aligned}
B_{21} &= \sum_{j=1}^{n}\left(\int_0^1 a_1\psi_j''\phi_2''dx\right)\hat{V}_j \\
&= \hat{V}_1\int_0^1 a_1\psi_1''\phi_2''dx + \hat{V}_2\int_0^1 a_1\psi_2''\phi_2''dx \\
&= \hat{V}_1\int_{I_2} a_1\psi_1''\phi_2''dx + \hat{V}_2\int_{I_2} a_1\psi_2''\phi_2''dx \\
&= \hat{V}_1\frac{h}{6}\left[a_1(x_1)\psi_1''(x_1)\phi_2''(x_1) + 4a_1(x_{3/2})\psi_1''(x_{3/2})\phi_2''(x_{3/2}) + a_1(x_2)\psi_1''(x_2)\phi_2''(x_2)\right] \\
&\quad +\hat{V}_2\frac{h}{6}\left[a_1(x_1)\psi_2''(x_1)\phi_2''(x_1) + 4a_1(x_{3/2})\psi_2''(x_{3/2})\phi_2''(x_{3/2}) + a_1(x_2)\psi_2''(x_2)\phi_2''(x_2)\right] \\
&= \hat{V}_1\frac{h}{6}\left(-\frac{4}{h}\right)\left(\frac{6}{h^2}\right) + \hat{V}_2\frac{h}{6}\left(-\frac{2}{h}\right)\left(\frac{6}{h^2}\right) \\
&= \frac{2}{h^2}(-2\hat{V}_1 - \hat{V}_2).
\end{aligned}
$$

$$
\begin{aligned}
B_{22} &= \sum_{j=1}^{n}\left(\int_0^1 a_2\psi_j''\psi_2''dx\right)\hat{V}_j \\
&= \hat{V}_1\int_0^1 a_2\psi_1''\phi_2''dx+\hat{V}_2\int_0^1 a_2\psi_2''\phi_2''dx+\hat{V}_3\int_0^1 a_2\psi_3''\phi_2''dx \\
&= \hat{V}_1\int_{I_2} a_2\psi_1''\phi_1''dx+\hat{V}_2\int_{I_2} a_2\psi_2''\phi_2''dx+\hat{V}_3\int_{I_3} a_2\psi_2''\phi_2''dx+\hat{V}_3\int_{I_3} a_2\psi_3''\phi_2''dx \\
&= \hat{V}_1\frac{h}{6}\left[a_2(x_1)\psi_1''(x_1)\phi_2''(x_1)+4a_2(x_{3/2})\psi_1''(x_{3/2})\phi_2''(x_{3/2})+a_2(x_2)\psi_1''(x_2)\phi_2''(x_2)\right]+ \\
&\quad \hat{V}_2\frac{h}{6}\left[a_2(x_1)\psi_2''(x_1)\phi_2''(x_1)+4a_2(x_{3/2})\psi_2''(x_{3/2})\phi_2''(x_{3/2})+a_2(x_2)\psi_2''(x_2)\phi_2''(x_2)\right]+ \\
&\quad \hat{V}_2\frac{h}{6}\left[a_2(x_2)\psi_2''(x_2)\phi_2''(x_2)+4a_2(x_{5/2})\psi_2''(x_{5/2})\phi_2''(x_{5/2})+a_2(x_3)\psi_2''(x_3)\phi_2''(x_3)\right]+ \\
&\quad \hat{V}_3\frac{h}{6}\left[a_2(x_2)\psi_3''(x_2)\phi_2''(x_2)+4a_2(x_{5/2})\psi_3''(x_{5/2})\phi_2''(x_{5/2})+a_2(x_3)\psi_3''(x_3)\phi_2''(x_3)\right] \\
&= \hat{V}_1\frac{h}{6}\left(\frac{2}{h}\right)\left(-\frac{6}{h^2}\right)+\hat{V}_2\frac{h}{6}\left(\frac{4}{h}\right)\left(-\frac{6}{h^2}\right)+\hat{V}_2\frac{h}{6}\left(-\frac{4}{h}\right)\left(-\frac{6}{h^2}\right)+\hat{V}_3\frac{h}{6}\left(-\frac{2}{h}\right)\left(-\frac{6}{h^2}\right) \\
&= \frac{2}{h^2}\left(-\hat{V}_1+\hat{V}_3\right).
\end{aligned}
$$

$$
\begin{aligned}
B_{23} &= \sum_{j=1}^{n}\left(\int_0^1 a_3\psi_j''\psi_2''dx\right)\hat{V}_j \\
&= \hat{V}_2\int_0^1 a_3\psi_2''\phi_2''dx+\hat{V}_3\int_0^1 a_3\psi_3''\phi_2''dx \\
&= \hat{V}_2\int_{I_3} a_3\psi_2''\phi_2''dx+\hat{V}_3\int_{I_3} a_3\psi_3''\phi_2''dx \\
&= \hat{V}_2\frac{h}{6}\left[a_3(x_2)\psi_2''(x_2)\phi_2''(x_2)+4a_3(x_{5/2})\psi_2''(x_{5/2})\phi_2''(x_{5/2})+a_3(x_3)\psi_2''(x_3)\phi_2''(x_3)\right]+ \\
&\quad \hat{V}_3\frac{h}{6}\left[a_3(x_2)\psi_3''(x_2)\phi_2''(x_2)+4a_3(x_{5/2})\psi_3''(x_{5/2})\phi_2''(x_{5/2})+a_3(x_3)\psi_3''(x_3)\phi_2''(x_3)\right] \\
&= \hat{V}_2\frac{h}{6}\left(\frac{2}{h}\right)\left(\frac{6}{h^2}\right)+\hat{V}_3\frac{h}{6}\left(\frac{4}{h}\right)\left(\frac{6}{h^2}\right) \\
&= \frac{2}{h^2}\left(\hat{V}_2+2\hat{V}_3\right). \\
B_{2k} &= 0 \quad \text{for } k\geq 4.
\end{aligned}
$$

Furthermore, it can be shown that this pattern goes on until the row $n-1$:

$$\begin{aligned}
B_{n-1,k} &= 0 \text{ for } k \leq n-3 \\
B_{n-1,n-2} &= \frac{2}{h^2}(-2\hat{V}_{n-2} - \hat{V}_{n-1}) \\
B_{n-1,n-1} &= \frac{2}{h^2}(-\hat{V}_{n-2} + \hat{V}_n) \\
B_{n-1,n} &= \frac{2}{h^2}(V_{n-1} + 2\hat{V}_n) \\
B_{n-1,n+1} &= 0.
\end{aligned}$$

For the last row, the nth row,

$$\begin{aligned}
B_{n,k} &= 0 \text{ for } k \leq n-2 \\
B_{n,n-1} &= \sum_{j=1}^{n} \left(\int_0^1 a_{n-1} \psi_j'' \phi_n'' dx \right) V_j' \\
&= \hat{V}_{n-1} \int_0^1 a_{n-1} \psi_{n-1}'' \phi_n'' dx + \hat{V}_n \int_0^1 a_{n-1} \psi_n'' \phi_n'' dx \\
&= \hat{V}_{n-1} \int_{I_n} a_{n-1} \psi_{n-1}'' \phi_n'' dx + \hat{V}_n \int_{I_n} a_{n-1} \psi_n'' \phi_n'' dx \\
&= \hat{V}_{n-1} \frac{h}{6} \left[a_{n-1}(x_{n-1}) \psi_{n-1}''(x_{n-1}) \phi_n''(x_{n-1}) + 4a_{n-1}(x_{n-1/2}) \psi_{n-1}''(x_{n-1/2}) \phi_n''(x_{n-1/2}) \right. \\
&\quad \left. + a_{n-1}(x_n) \psi_{n-1}''(x_n) \phi_n''(x_n) \right] + \\
&\quad \hat{V}_n \frac{h}{6} \left[a_{n-1}(x_{n-1}) \psi_n''(x_{n-1}) \phi_n''(x_{n-1}) + 4a_{n-1}(x_{n-1/2}) \psi_n''(x_{n-1/2}) \phi_n''(x_{n-1/2}) \right. \\
&\quad \left. + a_{n-1}(x_n) \psi_n''(x_n) \phi_n''(x_n) \right] \\
&= \hat{V}_{n-1} \frac{h}{6} \left(-\frac{4}{h} \right) \left(\frac{6}{h^2} \right) + \hat{V}_n \frac{h}{6} \left(-\frac{2}{h} \right) \left(\frac{6}{h^2} \right) \\
&= \frac{2}{h^2} \left(-2\hat{V}_{n-1} - \hat{V}_n \right)
\end{aligned}$$

$$
\begin{aligned}
B_{n,n} &= \sum_{j=1}^{n}\left(\int_0^1 a_n \psi_j'' \psi_n'' dx\right) V_j' \\
&= \hat{V}_{n-1}\int_0^1 a_n \psi_{n-1}''\phi_n'' dx + \hat{V}_n \int_0^1 a_n \psi_n'' \phi_n'' dx \\
&= \hat{V}_{n-1}\int_{I_n} a_n \psi_{n-1}''\phi_n'' dx + \hat{V}_n \int_{I_n} a_n \psi_n'' \phi_n'' dx + \hat{V}_n \int_{I_{n+1}} a_n \psi_n'' \phi_n'' dx \\
&= \hat{V}_{n-1}\frac{h}{6}\left[a_n(x_{n-1})\psi_{n-1}''(x_{n-1})\phi_n''(x_{n-1}) + 4a_n(x_{n-1/2})\psi_{n-1}''(x_{n-1/2})\phi_n''(x_{n-1/2})\right. \\
&\quad \left. + a_n(x_n)\psi_{n-1}''(x_n)\phi_n''(x_n)\right] \\
&\quad + \hat{V}_n\frac{h}{6}\left[a_n(x_{n-1})\psi_n''(x_{n-1})\phi_n''(x_{n-1}) + 4a_n(x_{n-1/2})\psi_n''(x_{n-1/2})\phi_n''(x_{n-1/2})\right. \\
&\quad \left. + a_n(x_n)\psi_n''(x_n)\phi_n''(x_n)\right] \\
&\quad + \hat{V}_n\frac{h}{6}\left[a_n(x_n)\psi_n''(x_n)\phi_n''(x_n) + 4a_n(x_{n+1/2})\psi_n''(x_{n+1/2})\phi_n''(x_{n+1/2})\right. \\
&\quad \left. + a_n(x_{n+1})\psi_n''(x_{n+1})\phi_n''(x_{n+1})\right] \\
&= \hat{V}_{n-1}\frac{h}{6}\left(\frac{2}{h}\right)\left(-\frac{6}{h^2}\right) + \hat{V}_n\frac{h}{6}\left(\frac{4}{h}\right)\left(-\frac{6}{h^2}\right) + \hat{V}_n\frac{h}{6}\left(-\frac{4}{h}\right)\left(-\frac{6}{h^2}\right) \\
&= -\frac{2}{h^2}\hat{V}_{n-1}
\end{aligned}
$$

$$
\begin{aligned}
B_{n,n+1} &= \sum_{j=1}^{n}\left(\int_0^1 a_{n+1} \psi_j'' \psi_n'' dx\right) V_j' \\
&= \hat{V}_n \int_0^1 a_{n+1}\psi_n''\phi_n'' dx \\
&= \hat{V}_n \int_{I_{n+1}} a_{n+1}\psi_n''\phi_n'' dx \\
&= \hat{V}_n\frac{h}{6}\left[a_{n+1}(x_n)\psi_n''(x_n)\phi_n''(x_n) + 4a_{n+1}(x_{n+1/2})\psi_n''(x_{n+1/2})\phi_n''(x_{n+1/2})\right. \\
&\quad \left. + a_{n+1}(x_{n+1})\psi_n''(x_{n+1})\phi_n''(x_{n+1})\right] \\
&= \hat{V}_n\frac{h}{6}\left(\frac{2}{h}\right)\left(\frac{6}{h^2}\right) \\
&= \frac{2}{h^2}\hat{V}_n
\end{aligned}
$$

This will produce the following matrix:

$$B = \frac{2}{h^2}\begin{pmatrix} -\hat{V}_1 & \hat{V}_2 & \hat{V}_1+2\hat{V}_2 & 0 & 0 & \dots & 0 \\ 0 & -2\hat{V}_1-\hat{V}_2 & -\hat{V}_1+\hat{V}_3 & \hat{V}_2+2\hat{V}_3 & 0 & \dots & 0 \\ 0 & 0 & -2\hat{V}_2-\hat{V}_3 & -\hat{V}_2+\hat{V}_4 & \hat{V}_3+2\hat{V}_4 & \dots & 0 \\ & & & \vdots & & & \\ 0 & \dots & 0 & -2\hat{V}_{n-2}-\hat{V}_{n-1} & -\hat{V}_{n-2}+\hat{V}_n & \hat{V}_{n-1}+2\hat{V}_n & 0 \\ 0 & \dots & 0 & 0 & -2\hat{V}_{n-1}-\hat{V}_n & -\hat{V}_{n-1} & \hat{V}_n \end{pmatrix}.$$

Now for the entries of the matrix D

$$\begin{aligned}
D_{ik} &= \sum_{j=1}^{n}\left(\int_0^1 a_k\phi_j''\psi_i''dx\right)V_j \text{ for } i=1,..,n \text{ and } k=0,...n+1. \\
D_{10} &= \sum_{j=1}^{n}\left(\int_0^1 a_0\phi_j''\psi_1''dx\right)V_j \\
&= V_1\int_{I_1} a_0\phi_1''\psi_1''dx \\
&= V_1\frac{h/2}{3}\left[a_0(x_0)\phi_1''(x_0)\psi_1''(x_0)+4a_0(x_{1/2})\phi_1''(x_{1/2})\psi_1''(x_{1/2})+a_0(x_1)\phi_1''(x_1)\psi_1''(x_1)\right] \\
&= V_1\frac{h}{6}\left[\left(\frac{6}{h^2}\right)\left(-\frac{2}{h}\right)\right] \\
&= \frac{2}{h^2}V_1.
\end{aligned}$$

$$\begin{aligned}
D_{11} &= \sum_{j=1}^{n}\left(\int_0^1 a_1\phi_j''\psi_1''dx\right)V_j \\
&= V_1\int_0^1 a_1\phi_1''\psi_1''dx+V_2\int_0^1 a_1\phi_2''\psi_1''dx \\
&= V_1\int_{I_1} a_1\phi_1''\psi_1''dx+V_1\int_{I_2} a_1\phi_1''\psi_1''dx+V_2\int_{I_2} a_1\phi_2''\psi_1''dx \\
&= V_1\frac{h}{6}\left[a_1(x_0)\phi_1''(x_0)\psi_1''(x_0)+4a_1(x_{1/2})\phi_1''(x_{1/2})\psi_1''(x_{1/2})+a_1(x_1)\phi_1''(x_1)\psi_1''(x_1)\right]+ \\
&\quad V_1\frac{h}{6}\left[a_1(x_1)\phi_1''(x_1)\psi_1''(x_1)+4a_1(x_{3/2})\phi_1''(x_{3/2})\psi_1''(x_{3/2})+a_1(x_2)\phi_1''(x_2)\psi_1''(x_2)\right]+ \\
&\quad V_2\frac{h}{6}\left[a_1(x_1)\phi_2''(x_1)\psi_1''(x_1)+4a_1(x_{3/2})\phi_2''(x_{3/2})\psi_1''(x_{3/2})+a_1(x_2)[\phi_2''(x_2)\psi_1''(x_2)]\right] \\
&= V_1\frac{h}{6}\left(-\frac{6}{h^2}\right)\left(\frac{4}{h^2}\right)+V_1\frac{h}{6}\left(-\frac{6}{h^2}\right)\left(-\frac{4}{h^2}\right)+V_2\frac{h}{6}\left(\frac{6}{h^2}\right)\left(-\frac{4}{h^2}\right) \\
&= -\frac{4}{h^2}V_2.
\end{aligned}$$

$$
\begin{aligned}
D_{12} &= \sum_{j=1}^{n}\left(\int_0^1 a_2\phi_j''\psi_1''dx\right)V_j \\
&= V_1\int_0^1 a_2\phi_1''\psi_1''dx + V_2\int_0^1 a_2\phi_2''\psi_1''dx \\
&= V_1\int_{I_2} a_2\phi_1''\psi_1''dx + V_2\int_{I_2} a_2\phi_2''\psi_1''dx \\
&= V_1\frac{h}{6}\left[a_2(x_1)\phi_1''(x_1)\psi_1''(x_1)+4a_2(x_{3/2})\phi_1''(x_{3/2})\psi_1''(x_{3/2})+a_2(x_2)\phi_1''(x_2)\psi_1''(x_2)\right]+ \\
&\quad V_2\frac{h}{6}\left[a_2(x_1)\phi_2''(x_1)\psi_1''(x_1)+4a_2(x_{3/2})\phi_2''(x_{3/2})\psi_1''(x_{3/2})+a_2(x_2)\phi_2''(x_2)\psi_1''(x_2)\right] \\
&= V_1\frac{h}{6}\left(\frac{6}{h^2}\right)\left(\frac{2}{h}\right)+V_2\frac{h}{6}\left(-\frac{6}{h^2}\right)\left(\frac{2}{h}\right) \\
&= \frac{2}{h^2}(V_1-V_2) \\
D_{1k} &= 0 \text{ for } k\geq 3.
\end{aligned}
$$

Now let's look at the 2nd row

$$
\begin{aligned}
D_{20} &= 0. \\
D_{21} &= \sum_{j=1}^{n}\left(\int_0^1 a_1\phi_j''\psi_2''dx\right)V_j \\
&= V_1\int_0^1 a_1\phi_1''\psi_2''dx + V_2\int_0^1 a_1\phi_2''\psi_2''dx \\
&= V_1\int_{I_2} a_1\phi_1''\psi_2''dx + V_2\int_{I_2} a_1\phi_2''\psi_2''dx \\
&= V_1\frac{h}{6}\left[a_1(x_1)\phi_1''(x_1)\psi_2''(x_1)+4a_1(x_{3/2})\phi_1''(x_{3/2})\psi_2''(x_{3/2})+a_1(x_2)\phi_1''(x_2)\psi_2''(x_2)\right]+ \\
&\quad V_2\frac{h}{6}\left[a_1(x_1)\phi_2''(x_1)\psi_2''(x_1)+4a_1(x_{3/2})\phi_2''(x_{3/2})\psi_2''(x_{3/2})+a_1(x_2)\phi_2''(x_2)\psi_2''(x_2)\right] \\
&= V_1\frac{h}{6}\left[\left(-\frac{6}{h^2}\right)\left(-\frac{2}{h}\right)\right]+V_2\frac{h}{6}\left[\left(\frac{6}{h^2}\right)\left(-\frac{2}{h}\right)\right] \\
&= \frac{2}{h^2}(V_1-V_2).
\end{aligned}
$$

$$
\begin{aligned}
D_{22} &= \sum_{j=1}^{n}\left(\int_0^1 a_2\phi_j''\psi_2''dx\right)V_j \\
&= V_1\int_0^1 a_2\phi_1''\psi_2''dx + V_2\int_0^1 a_2\phi_2''\psi_2''dx + V_3\int_0^1 a_2\phi_3''\psi_2''dx \\
&= V_1\int_{I_2} a_2\phi_1''\psi_2''dx + V_2\int_{I_2} a_2\phi_2''\psi_2''dx + V_2\int_{I_3} a_2\phi_2''\psi_2''dx + V_3\int_{I_3} a_2\phi_3''\psi_2''dx \\
&= V_1\frac{h}{6}\left[a_2(x_1)\phi_1''(x_1)\psi_2''(x_1) + 4a_2(x_{3/2})\phi_1''(x_{3/2})\psi_2''(x_{3/2}) + a_2(x_2)\phi_1''(x_2)\psi_2''(x_2)\right] + \\
&\quad V_2\frac{h}{6}\left[a_2(x_1)\phi_2''(x_1)\psi_2''(x_1) + 4a_2(x_{3/2})\phi_2''(x_{3/2})\psi_2''(x_{3/2}) + a_2(x_2)\phi_2''(x_2)\psi_2''(x_2)\right] + \\
&\quad V_2\frac{h}{6}\left[a_2(x_2)\phi_2''(x_2)\psi_2''(x_2) + 4a_2(x_{5/2})\phi_2''(x_{5/2})\psi_2''(x_{5/2}) + a_2(x_3)\phi_2''(x_3)\psi_2''(x_3)\right] + \\
&\quad V_3\frac{h}{6}\left[a_2(x_2)\phi_3''(x_2)\psi_2''(x_2) + 4a_2(x_{5/2})\phi_3''(x_{5/2})\psi_2''(x_{5/2}) + a_2(x_3)\phi_3''(x_3)\psi_2''(x_3)\right] \\
&= V_1\frac{h}{6}\left(\frac{6}{h^2}\right)\left(\frac{4}{h^2}\right) + V_2\frac{h}{6}\left(-\frac{6}{h^2}\right)\left(\frac{4}{h^2}\right) + V_2\frac{h}{6}\left(-\frac{6}{h^2}\right)\left(-\frac{4}{h^2}\right) + V_3\frac{h}{6}\left(\frac{6}{h^2}\right)\left(-\frac{4}{h^2}\right) \\
&= \frac{2}{h^2}(2V_1 - 2V_3).
\end{aligned}
$$

$$
\begin{aligned}
D_{23} &= \sum_{j=1}^{n}\left(\int_0^1 a_3\phi_j''\psi_2''dx\right)V_j \\
&= V_2\int_0^1 a_3\phi_2''\psi_2''dx + V_3\int_0^1 a_3\phi_3''\psi_2''dx \\
&= V_2\int_{I_3} a_3\phi_2''\psi_2''dx + V_3\int_{I_3} a_3\phi_3''\psi_2''dx \\
&= V_2\frac{h}{6}\left[a_3(x_2)\phi_2''(x_2)\psi_2''(x_2) + 4a_3(x_{5/2})\phi_2''(x_{5/2})\psi_2''(x_{5/2}) + a_3(x_3)\phi_2''(x_3)\psi_2''(x_3)\right] + \\
&\quad V_3\frac{h}{6}\left[a_3(x_2)\phi_3''(x_2)\psi_2''(x_2) + 4a_3(x_{5/2})\phi_3''(x_{5/2})\psi_2''(x_{5/2}) + a_3(x_3)\phi_3''(x_3)\psi_2''(x_3)\right] \\
&= V_2\frac{h}{6}\left(\frac{6}{h^2}\right)\left(\frac{2}{h}\right) + V_3\frac{h}{6}\left(-\frac{6}{h^2}\right)\left(\frac{2}{h}\right) \\
&= \frac{2}{h^2}(V_2 - V_3) \\
D_{2k} &= 0 \text{ for } k \geq 4.
\end{aligned}
$$

It can be shown that this pattern goes on until the $N-1$-st row,

$$\begin{aligned}
D_{n-1,k} &= 0 \text{ for } k \le n-3 \\
D_{n-1,n-2} &= \frac{2}{h^2}(V_{n-2}-V_{n-1}) \\
D_{n-1,n-1} &= \frac{2}{h^2}(2V_{n-2}-2V_n) \\
D_{n-1,n} &= \frac{2}{h^2}(V_{n-1}-V_n) \\
D_{n-1,n+1} &= 0.
\end{aligned}$$

For the last row, the n-th row,

$$\begin{aligned}
D_{n,k} &= 0 \text{ for } k \le n-2 \\
D_{n,n-1} &= \sum_{j=1}^{n}\left(\int_0^1 a_{n-1}\phi_j''\psi_n''dx\right)V_j \\
&= V_{n-1}\int_0^1 a_{n-1}\phi_{n-1}''\psi_n''dx + V_n\int_0^1 a_{n-1}\phi_n''\psi_n''dx \\
&= V_{n-1}\int_{I_n} a_{n-1}\phi_{n-1}''\psi_n''dx + V_n\int_{I_n} a_{n-1}\phi_n''\psi_n''dx \\
&= V_{n-1}\frac{h}{6}\left[a_{n-1}(x_{n-1})\phi_{n-1}''(x_{n-1})\psi_n''(x_{n-1}) + 4a_{n-1}(x_{n-1/2})\phi_{n-1}''(x_{n-1/2})\psi_n''(x_{n-1/2})\right. \\
&\quad \left. + a_{n-1}(x_n)\phi_{n-1}''(x_n)\psi_n''(x_n)\right] \\
&\quad + V_n\frac{h}{6}\left[a_{n-1}(x_{n-1})\phi_n''(x_{n-1})\psi_n''(x_{n-1})\right. \\
&\quad \left. + 4a_{n-1}(x_{3/2})\phi_n''(x_{n-1/2})\psi_n''(x_{n-1/2}) + a_{n-1}(x_n)\phi_n''(x_n)\psi_n''(x_n)\right] \\
&= V_{n-1}\frac{h}{6}\left[\left(-\frac{6}{h^2}\right)\left(-\frac{2}{h}\right)\right] + V_n\frac{h}{6}\left[\left(\frac{6}{h^2}\right)\left(-\frac{2}{h}\right)\right] \\
&= \frac{2}{h^2}(V_{n-1}-V_n).
\end{aligned}$$

$$
\begin{aligned}
D_{n,n} &= \sum_{j=1}^{n}\left(\int_0^1 a_n\phi_j''\psi_n''dx\right)V_j \\
&= V_{n-1}\int_0^1 a_n\phi_{n-1}''\psi_n''dx + V_n\int_0^1 a_n\phi_n''\psi_n''dx \\
&= V_{n-1}\int_{I_n} a_n\phi_{n-1}''\psi_n''dx + V_n\int_{I_n} a_n\phi_n''\psi_n''dx + V_n\int_{I_{n+1}} a_n\phi_n''\psi_n''dx + \\
&= V_{n-1}\frac{h}{6}\left[a_n(x_{n-1})\phi_{n-1}''(x_{n-1})\psi_n''(x_{n-1})\right. \\
&\quad \left.+4a_n(x_{n-1/2})\phi_{n-1}''(x_{n-1/2})\psi_n''(x_{n-1/2}) + a_n(x_n)\phi_{n-1}''(x_n)\psi_n''(x_n)\right] \\
&\quad +V_n\frac{h}{6}\left[a_n(x_{n-1})\phi_n''(x_{n-1})\psi_n''(x_{n-1})\right. \\
&\quad \left.+4a_n(x_{n-1/2})\phi_n''(x_{n-1/2})\psi_n''(x_{n-1/2}) + a_n(x_n)\phi_n''(x_n)\psi_n''(x_n)\right] \\
&\quad +V_n\frac{h}{6}\left[a_n(x_n)\phi_n''(x_n)\psi_n''(x_n) + 4a_n(x_{n+1/2})\phi_n''(x_{n+1/2})\psi_n''(x_{n+1/2})\right. \\
&\quad \left.+a_n(x_{n+1})\phi_n''(x_{n+1})\psi_n''(x_{n+1})\right] \\
&= V_{n-1}\frac{h}{6}\left(\frac{6}{h^2}\right)\left(\frac{4}{h^2}\right) + V_n\frac{h}{6}\left(-\frac{6}{h^2}\right)\left(\frac{4}{h^2}\right) + V_n\frac{h}{6}\left(-\frac{6}{h^2}\right)\left(-\frac{4}{h^2}\right) \\
&= \frac{2}{h^2}\cdot 2V_{n-1}.
\end{aligned}
$$

$$
\begin{aligned}
D_{n,n+1} &= \sum_{j=1}^{n}\left(\int_0^1 a_{n+1}\phi_j''\psi_n''dx\right)V_j \\
&= V_n\int_0^1 a_{n+1}\phi_n''\psi_n''dx \\
&= V_n\int_{I_{n+1}} a_{n+1}\phi_n''\psi_n''dx \\
&= V_n\frac{h}{6}\left[a_{n+1}(x_n)\phi_n''(x_n)\psi_n''(x_n) + 4a_{n+1}(x_{n+1/2})\phi_n''(x_{n+1/2})\psi_n''(x_{n+1/2})\right. \\
&\quad \left.+a_{n+1}(x_{n+1})\phi_n''(x_{n+1})\psi_n''(x_{n+1})\right] \\
&= V_n\frac{h}{6}\left(\frac{6}{h^2}\right)\left(\frac{2}{h}\right) \\
&= \frac{2}{h^2}\cdot V_n.
\end{aligned}
$$

Putting the entries together we get

$$D = \frac{2}{h^2}\begin{pmatrix} -V_1 & -2V_2 & V_1 - V_2 & 0 & 0 & \dots & 0 \\ 0 & V_1 - V_2 & 2V_1 - 2V_3 & V_2 - V_3 & 0 & \dots & 0 \\ 0 & \dots & V_2 - V_3 & -V_2 - 2V_4 & V_3 - V_4 & \dots & 0 \\ & & & \vdots & & & \\ 0 & \dots & 0 & V_{\text{n-2}} - V_{\text{n-1}} & 2V_{\text{n-2}} - 2V_n & V_{\text{n-1}} - V_n & 0 \\ 0 & \dots & 0 & 0 & V_{\text{n-1}} - V_n & 2V_{\text{n-1}} & V_n \end{pmatrix}.$$

Now for the entries of the C matrix we have the formula

$$\begin{aligned} C_{ik} &= \sum_{j=1}^{n}\left(\int_0^1 a_k \psi_j'' \psi_i'' dx\right)\hat{V}_j \text{ for } i = 1,..,n \text{ and } k = 0,...n+1. \\ Therefore, C_{10} &= \sum_{j=1}^{n}\left(\int_0^1 a_0 \psi_j'' \psi_1'' dx\right)\hat{V}_j \\ &= \hat{V}_1 \int_{I_1} a_0 \left(\psi_1''\right)^2 dx \\ &= \hat{V}_1 \frac{h/2}{3}\left[a_0(x_0)\left(\psi_1''(x_0)\right)^2 + 4a_0(x_{1/2})\left(\psi_1''(x_{1/2})\right)^2 + a_0(x_1)\left(\psi_1''(x_1)\right)^2\right] \\ &= \hat{V}_1 \frac{h}{6}\left[\left(-\frac{2}{h}\right)^2 + 4\left(\frac{1}{2}\right)\left(\frac{1}{h}\right)^2 + 0\right] \\ &= \hat{V}_1 \frac{h}{6}\left[\frac{4}{h^2} + \frac{2}{h^2}\right] \\ &= \frac{1}{h}\hat{V}_1. \end{aligned}$$

$$
\begin{aligned}
C_{11} &= \sum_{j=1}^{n}\left(\int_0^1 a_1\psi_j''\psi_1''dx\right)V_j' \\
&= \hat{V}_1\int_0^1 a_1(\psi_1'')^2dx+\hat{V}_2\int_0^1 a_1\psi_2''\psi_1''dx \\
&= \hat{V}_1\int_{I_1} a_1(\psi_1'')^2dx+\hat{V}_1\int_{I_2} a_1(\psi_1'')^2dx+\hat{V}_2\int_{I_2} a_1\psi_2''\psi_1''dx \\
&= \hat{V}_1\frac{h}{6}\left[a_1(x_0)\left(\psi_1''(x_0)\right)^2+4a_1(x_{1/2})\left(\psi_1''(x_{1/2})\right)^2+a_1(x_1)\left(\psi_1''(x_1)\right)^2\right]+ \\
&\quad \hat{V}_1\frac{h}{6}\left[a_1(x_1)\left(\psi_1''(x_1)\right)^2+4a_1(x_{3/2})\left(\psi_1''(x_{3/2})\right)^2+a_1(x_2)\left(\psi_1''(x_2)\right)^2\right]+ \\
&\quad \hat{V}_2\frac{h}{6}\left[a_1(x_1)\psi_2''(x_1)\psi_1''(x_1)+4a_1(x_{3/2})\psi_2''(x_{3/2})\psi_1''(x_{3/2})+a_1(x_2)\psi_2''(x_2)\psi_1''(x_2)\right] \\
&= \hat{V}_1\frac{h}{6}\left[4\left(\frac{1}{2}\right)\left(\frac{1}{h}\right)^2+\left(\frac{4}{h}\right)^2\right]+\hat{V}_1\frac{h}{6}\left[\left(-\frac{4}{h}\right)^2+4\left(\frac{1}{2}\right)\left(-\frac{1}{h}\right)^2\right]+ \\
&\quad \hat{V}_2\frac{h}{6}\left[\left(-\frac{2}{h}\right)\left(-\frac{4}{h}\right)+4\left(\frac{1}{2}\right)\left(\frac{1}{h}\right)\left(-\frac{1}{h}\right)\right] \\
&= \hat{V}_1\frac{h}{6}\left[\frac{2}{h^2}+\frac{16}{h^2}+\frac{16}{h^2}+\frac{2}{h^2}\right]+\hat{V}_2\frac{h}{6}\left[\frac{8}{h^2}+\frac{-2}{h^2}\right] \\
&= \hat{V}_1\frac{h}{6}\left[\frac{36}{h^2}\right]+\hat{V}_2\frac{h}{6}\left[\frac{6}{h^2}\right] \\
&= \frac{1}{h}\left(6\hat{V}_1+\hat{V}_2\right). \\
C_{12} &= \sum_{j=1}^{n}\left(\int_0^1 a_2\psi_j''\psi_1''dx\right)V_j \\
&= \hat{V}_1\int_0^1 a_2\left(\psi_1''\right)^2dx+\hat{V}_2\int_0^1 a_2\psi_2''\psi_1''dx \\
&= \hat{V}_1\int_{I_2} a_2\left(\psi_1''\right)^2dx+\hat{V}_2\int_{I_2} a_2\psi_2''\psi_1''dx \\
&= \hat{V}_1\frac{h}{6}\left[a_2(x_1)\left(\psi_1''(x_1)\right)^2+4a_2(x_{3/2})\left(\psi_1''(x_{3/2})\right)^2+a_2(x_2)\left(\psi_1''(x_2)\right)^2\right]+ \\
&\quad \hat{V}_2\frac{h}{6}\left[a_2(x_1)\psi_2''(x_1)\psi_1''(x_1)+4a_2(x_{3/2})\psi_2''(x_{3/2})\psi_1''(x_{3/2})+a_2(x_2)\psi_2''(x_2)\psi_1''(x_2)\right] \\
&= \hat{V}_1\frac{h}{6}\left[4\frac{1}{2}\left(-\frac{1}{h}\right)^2+\left(\frac{2}{h}\right)^2\right]+\hat{V}_2\frac{h}{6}\left[4\frac{1}{2}\left(\frac{1}{h}\right)\left(-\frac{1}{h}\right)+\left(\frac{4}{h}\right)\left(\frac{2}{h}\right)\right] \\
&= \hat{V}_1\frac{h}{6}\left[\frac{2}{h^2}+\frac{4}{h^2}\right]+\hat{V}_2\frac{h}{6}\left[-\frac{2}{h^2}+\frac{8}{h^2}\right] \\
&= \frac{1}{h}\left(\hat{V}_1+\hat{V}_2\right). \\
C_{1k} &= 0 \text{ for } k\geq 3.
\end{aligned}
$$

Now we look at the second row:

$$
\begin{aligned}
C_{20} &= 0. \\
C_{21} &= \sum_{j=1}^{n}\left(\int_0^1 a_1\psi_j''\psi_2''dx\right)V_j' \\
&= V_1\int_0^1 a_1\psi_1''\psi_2''dx + V_2\int_0^1 a_1(\psi_2'')^2dx \\
&= V_1\int_{I_2} a_1\psi_1''\psi_2''dx + V_2\int_{I_2} a_1(\psi_2'')^2dx \\
&= \hat{V}_1\frac{h}{6}[a_1(x_1)\psi_1''(x_1)\psi_2''(x_1) + 4a_1(x_{3/2})\psi_1''(x_{3/2})\psi_2''(x_{3/2}) + a_1(x_2)\psi_1''(x_2)\psi_2''(x_2)] \\
&\quad +\hat{V}_2\frac{h}{6}[a_1(x_1)[\psi_2''(x_1)]^2 + 4a_1(x_{3/2})[\psi_2''(x_{3/2})]^2 + a_1(x_2)[\psi_2''(x_2)]^2] \\
&= \hat{V}_1\frac{h}{6}\left[\left(\frac{-4}{h}\right)\left(\frac{-2}{h}\right) + 4\left(\frac{1}{2}\right)\left(\frac{-1}{h}\right)\left(\frac{1}{h}\right)\right] + \hat{V}_2\frac{h}{6}\left[\left(\frac{-2}{h}\right)^2 + 4\left(\frac{1}{2}\right)\left(\frac{1}{h}\right)^2\right] \\
&= \hat{V}_1\frac{h}{6}\left[\frac{8}{h^2} + \frac{-2}{h^2}\right] + \hat{V}_2\frac{h}{6}\left[\frac{4}{h^2} + \frac{2}{h^2}\right] \\
&= \frac{1}{h}\left(\hat{V}_1 + \hat{V}_2\right). \\
C_{22} &= \sum_{j=1}^{n}\left(\int_0^1 a_2\psi_j''\psi_2''dx\right)\hat{V}_j \\
&= \hat{V}_1\int_0^1 a_2\psi_1''\psi_2''dx + \hat{V}_2\int_0^1 a_2(\psi_2'')^2dx + \hat{V}_3\int_0^1 a_2\psi_3''\psi_2''dx \\
&= \hat{V}_1\int_{I_2} a_2\psi_1''\psi_2''dx + \hat{V}_2\int_{I_2} a_2(\psi_2'')^2dx + \hat{V}_2\int_{I_3} a_2(\psi_2'')^2dx + \hat{V}_3\int_{I_3} a_2\psi_3''\psi_2''dx \\
&= \hat{V}_1\frac{h}{6}\left[a_2(x_1)\psi_1''(x_1)\psi_2''(x_1) + 4a_2(x_{3/2})\psi_1''(x_{3/2})\psi_2''(x_{3/2}) + a_2(x_2)\psi_1''(x_2)\psi_2''(x_2)\right] + \\
&\quad \hat{V}_2\frac{h}{6}\left[a_2(x_1)(\psi_2''(x_1))^2 + 4a_2(x_{3/2})(\psi_2''(x_{3/2}))^2 + a_2(x_2)(\psi_2''(x_2))^2\right] + \\
&\quad \hat{V}_2\frac{h}{6}\left[a_2(x_2)(\psi_2''(x_2))^2 + 4a_2(x_{5/2})(\psi_2''(x_{5/2}))^2 + a_2(x_3)(\psi_2''(x_3))^2\right] + \\
&\quad \hat{V}_3\frac{h}{6}\left[a_2(x_2)\psi_3''(x_2)\psi_2''(x_2) + 4a_2(x_{5/2})\psi_3''(x_{5/2})\psi_2''(x_{5/2}) + a_2(x_3)\psi_3''(x_3)\psi_2''(x_3)\right] \\
&= \hat{V}_1\frac{h}{6}\left[4\left(\frac{1}{2}\right)\left(-\frac{1}{h}\right)\left(\frac{1}{h}\right) + \left(\frac{2}{h}\right)\left(\frac{4}{h}\right)\right] + \hat{V}_2\frac{h}{6}\left[4\left(\frac{1}{2}\right)\left(\frac{1}{h}\right)^2 + \left(\frac{4}{h}\right)^2\right] \\
&\quad +\hat{V}_2\frac{h}{6}\left[\left(-\frac{4}{h}\right)^2 + 4\left(\frac{1}{2}\right)\left(-\frac{1}{h}\right)^2\right] + \hat{V}_3\frac{h}{6}\left[\left(-\frac{2}{h}\right)\left(-\frac{4}{h}\right) + 4\left(\frac{1}{2}\right)\left(\frac{1}{h}\right)\left(-\frac{1}{h}\right)\right] \\
&= \hat{V}_1\frac{h}{6}\left[-\frac{2}{h^2} + \frac{8}{h^2}\right] + \hat{V}_2\frac{h}{6}\left[\frac{2}{h^2} + \frac{16}{h^2} + \frac{16}{h^2} + \frac{2}{h^2}\right] + \hat{V}_3\frac{h}{6}\left[\frac{8}{h^2} - \frac{2}{h^2}\right] \\
&= \hat{V}_1\frac{h}{6}\left[\frac{6}{h^2}\right] + \hat{V}_2\frac{h}{6}\left[\frac{36}{h^2}\right] + \hat{V}_3\frac{h}{6}\left[\frac{6}{h^2}\right].
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{1}{h}\left(\hat{V}_1 + 6\hat{V}_2 + \hat{V}_3\right). \\
C_{23} &= \sum_{j=1}^{n}\left(\int_0^1 a_3 \psi_j'' \psi_2'' dx\right)\hat{V}_j \\
&= \hat{V}_2 \int_0^1 a_3 (\psi_2'')^2 dx + \hat{V}_3 \int_0^1 a_3 \psi_3'' \psi_2'' dx \\
&= \hat{V}_2 \int_{I_3} a_3 (\psi_2'')^2 dx + \hat{V}_3 \int_{I_3} a_3 \psi_3'' \psi_2'' dx \\
&= \hat{V}_2 \frac{h}{6}\left[a_3(x_2)\psi_2''(x_2)^2 + 4a_3(x_{5/2})\psi_2''(x_{5/2})^2 + a_3(x_3)\psi_2''(x_3)^2\right] + \\
&\quad \hat{V}_3 \frac{h}{6}\left[a_3(x_2)\psi_3''(x_2)\psi_2''(x_2) + 4a_3(x_{5/2})\psi_3''(x_{5/2})\psi_2''(x_{5/2}) + a_3(x_3)\psi_3''(x_3)\psi_2''(x_3)\right] \\
&= \hat{V}_2 \frac{h}{6}\left[4\frac{1}{2}\left(-\frac{1}{h}\right)^2 + \left(\frac{2}{h}\right)^2\right] + \hat{V}_3 \frac{h}{6}\left[4\frac{1}{2}\left(\frac{1}{h}\right)\left(-\frac{1}{h}\right) + \left(\frac{4}{h}\right)\left(\frac{2}{h}\right)\right] \\
&= \hat{V}_2 \frac{h}{6}\left[\frac{2}{h^2} + \frac{4}{h^2}\right] + \hat{V}_3 \frac{h}{6}\left[-\frac{2}{h^2} + \frac{8}{h^2}\right] \\
&= \frac{1}{h}\left(\hat{V}_2 + \hat{V}_3\right) \\
C_{2k} &= 0 \text{ for } k \geq 4.
\end{aligned}
$$

It can be shown that this pattern goes on until the $n-1$ row,

$$
\begin{aligned}
C_{n-1,k} &= 0 \text{ for } k \leq n-3 \\
C_{n-1,n-2} &= \frac{1}{h}\left(\hat{V}_{n-2} + \hat{V}_{n-1}\right) \\
C_{n-1,n-1} &= \frac{1}{h}\left(\hat{V}_{n-2} + 6\hat{V}_{n-1} + \hat{V}_n\right) \\
C_{n-1,n} &= \frac{1}{h}\left(\hat{V}_{n-1} + \hat{V}_n\right) \\
C_{n-1,n+1} &= 0.
\end{aligned}
$$

For the last row, the n^{th} row,

$$
C_{n,k} = 0 \text{ for } k \leq n-2.
$$

$$
\begin{aligned}
C_{n,n-1} &= \sum_{j=1}^{n}\left(\int_0^1 a_{n-1}\psi_j''\psi_n''dx\right)\hat{V}_j \\
&= \hat{V}_{n-1}\int_0^1 a_{n-1}\psi_{n-1}''\psi_n''dx + V_n\int_0^1 a_{n-1}(\psi_n'')^2dx \\
&= \hat{V}_{n-1}\int_{I_n} a_{n-1}\psi_{n-1}''\psi_n''dx + V_n\int_{I_n} a_{n-1}(\psi_n'')^2dx \\
&= \hat{V}_{n-1}\frac{h}{6}[a_{n-1}(x_{n-1})\psi_{n-1}''(x_{n-1})\psi_n''(x_{n-1})] \\
&\quad +4a_{n-1}(x_{n-1/2})\psi_{n-1}''(x_{n-1/2})\psi_n''(x_{n-1/2}) + a_{n-1}(x_n)\psi_{n-1}''(x_n)\psi_n''(x_n)] \\
&\quad +\hat{V}_{n-1}\frac{h}{6}[a_{n-1}(x_{n-1})[\psi_n''(x_{n-1})]^2 + 4a_{n-1}(x_{n-1/2})[\psi_n''(x_{n-1/2})]^2 + a_{n-1}(x_n)[\psi_n''(x_n)]^2 \\
&= \hat{V}_{n-1}\frac{h}{6}\left[\left(-\frac{4}{h}\right)\left(-\frac{2}{h}\right)+4\left(\frac{1}{2}\right)\left(-\frac{1}{h}\right)\left(\frac{1}{h}\right)\right] + \hat{V}_n\frac{h}{6}\left[\left(\frac{-2}{h}\right)^2+4\left(\frac{1}{2}\right)\left(\frac{1}{h}\right)^2\right] \\
&= \hat{V}_{n-1}\frac{h}{6}\left[\frac{8}{h^2}-\frac{2}{h^2}\right] + \hat{V}_{n-1}\frac{h}{6}\left[\frac{4}{h^2}+\frac{2}{h^2}\right] \\
&= \frac{1}{h}\left(\hat{V}_{n-1}+\hat{V}_n\right). \\
C_{n,n} &= \sum_{j=1}^{n}\left(\int_0^1 a_2\psi_j''\psi_2''dx\right)\hat{V}_j \\
&= \hat{V}_{n-1}\int_0^1 a_n\psi_{n-1}''\psi_n''dx + \hat{V}_n\int_0^1 a_n\left(\psi_n''\right)^2dx \\
&= \hat{V}_{n-1}\int_{I_n} a_n\psi_{n-1}''\psi_n''dx + \hat{V}_n\int_{I_n} a_n\left(\psi_n''\right)^2dx + \hat{V}_n\int_{I_{n+1}} a_n\left(\psi_n''\right)^2dx \\
&= \hat{V}_{n-1}\frac{h}{6}\left[a_n(x_{n-1})\psi_{n-1}''(x_{n-1})\psi_n''(x_{n-1}) + 4a_n(x_{n-1/2})\psi_{n-1}''(x_{n-1/2})\psi_n''(x_{n-1/2})\right. \\
&\quad \left. +a_n(x_n)\psi_{n-1}''(x_n)\psi_n''(x_n)\right] + \hat{V}_n\frac{h}{6}\left[a_n(x_{n-1})\left(\psi_n''(x_{n-1})\right)^2\right. \\
&\quad \left. +4a_n(x_{n-1/2})\left(\psi_n''(x_{n-1/2})\right)^2 + a_n(x_n)\left(\psi_n''(x_n)\right)^2\right] + \hat{V}_n\frac{h}{6}\left[a_n(x_n)\left(\psi_n''(x_n)\right)^2\right. \\
&\quad \left. +4a_n(x_{n+1/2})\left(\psi_n''(x_{n+1/2})\right)^2 + a_n(x_{n+1})\left(\psi_n''(x_{n+1})\right)^2\right] \\
&= \hat{V}_{n-1}\frac{h}{6}\left[4\left(\frac{1}{2}\right)\left(-\frac{1}{h}\right)\left(\frac{1}{h}\right)+\left(\frac{2}{h}\right)\left(\frac{4}{h}\right)\right] + \hat{V}_n\frac{h}{6}\left[4\left(\frac{1}{2}\right)\left(\frac{1}{h}\right)^2+\left(\frac{4}{h}\right)^2\right] \\
&\quad +\hat{V}_n\frac{h}{6}\left[\left(-\frac{4}{h}\right)^2+4\left(\frac{1}{2}\right)\left(-\frac{1}{h}\right)^2\right] \\
&= \hat{V}_{n-1}\frac{h}{6}\left[-\frac{2}{h^2}+\frac{8}{h^2}\right] + \hat{V}_n\frac{h}{6}\left[\frac{2}{h^2}+\frac{16}{h^2}+\frac{16}{h^2}+\frac{2}{h^2}\right] \\
&= \hat{V}_{n-1}\frac{h}{6}\left[\frac{6}{h^2}\right] + \hat{V}_n\frac{h}{6}\left[\frac{36}{h^2}\right] \\
&= \frac{1}{h}\left(\hat{V}_{n-1}+6\hat{V}_n\right).
\end{aligned}
$$

$$
\begin{aligned}
C_{n,n+1} &= \sum_{j=1}^{n} \left(\int_0^1 a_{n+1} \psi_j'' \psi_n'' dx \right) \hat{V}_j \\
&= \hat{V}_n \int_0^1 a_{n+1} \left(\psi_n'' \right)^2 dx \\
&= \hat{V}_n \int_{I_{n+1}} a_{n+1} \left(\psi_n'' \right)^2 dx \\
&= \hat{V}_n \frac{h}{6} \left[a_{n+1}(x_n) \left(\psi_n''(x_n) \right)^2 + 4 a_{n+1}(x_{n+1/2}) \left(\psi_n''(x_{n+1/2}) \right)^2 + a_{n+1}(x_{n+1}) \left(\psi_n''(x_{n+1}) \right)^2 \right] \\
&= \hat{V}_n \frac{h}{6} \left[4 \frac{1}{2} \left(-\frac{1}{h} \right)^2 + \left(\frac{2}{h} \right)^2 \right] \\
&= \hat{V}_n \frac{h}{6} \left[\frac{2}{h^2} + \frac{4}{h^2} \right] \\
&= \frac{1}{h} \hat{V}_n.
\end{aligned}
$$

Collecting the entries of the matrix we get

$$
C = \frac{1}{h} \begin{pmatrix}
\hat{V}_1 & 6\hat{V}_1 + \hat{V}_2 & \hat{V}_1 + \hat{V}_2 & 0 & 0 & \dots & 0 \\
0 & \hat{V}_1 + \hat{V}_2 & \hat{V}_1 + 6\hat{V}_2 + \hat{V}_3 & \hat{V}_2 + \hat{V}_3 & 0 & \dots & 0 \\
0 & \dots & \hat{V}_2 + \hat{V}_3 & \hat{V}_2 + 6\hat{V}_3 + \hat{V}_4 & \hat{V}_3 + \hat{V}_4 & \dots & 0 \\
 & & & \vdots & & & \\
0 & \dots & 0 & \hat{V}_{n-2} + \hat{V}_{n-1} & \hat{V}_{n-2} + 6\hat{V}_{n-1} + \hat{V}_n & \hat{V}_{n-1} + \hat{V}_n & 0 \\
0 & \dots & 0 & 0 & \hat{V}_{n-1} + \hat{V}_n & \hat{V}_{n-1} + 6\hat{V}_n & \hat{V}_n
\end{pmatrix}.
$$

Chapter 6

Proximal Point Method

In this chapter we discuss various proximal point methods and employ them to solve the inverse problem of parameter identification in the fourth-order beam equation.

6.1 Optimization Formulation

We recall the optimization problem that we consider reads as:

$$\min_{a \in \tilde{A}} J(a). \tag{6.1}$$

We emphasize on two cases. The first case is of the output least squares (OLS) functional given by

$$J(a) = J_1(a) + R(a), \tag{6.2}$$

where

$$J_1(a) = \frac{1}{2}\|u(a) - z\|^2.$$

The second case is of the modified output least squares (OLS) functional given by

$$J(a) = J_2(a) + R(a), \tag{6.3}$$

where

$$J_2(a) = \frac{1}{2}T(a, u - z, u - z).$$

Recall the in the above $u(a)$ is a solution of the weak form, z is the data, and R is the regularization functional.

We consider the following three choices for R:

$$R(a) = R_1(a)\ (L_2\text{-norm}) \tag{6.4a}$$

$$R(a) = R_2(a)\ (H_1\text{-norm}) \tag{6.4b}$$

$$R(a) = R_3(a)\ (H_1\text{semi-norm}). \tag{6.4c}$$

We remark that the functional J_1 is not convex and the convexity can only be achieved by choosing a sufficiently large regularization parameter. On the other hand, J_2 is always convex. Due to the convexity, our most arguments are valid for J_2 only. Furthermore, all the numerical experiments are done for J_2 only. We choose the constraint set $\tilde{A}$ to be closed and convex.
We now describe the proximal point method:

$$\begin{aligned} a^{k+1} &= \min_{a\in\tilde{A}} \left\{ J(a) + \frac{1}{2\lambda^k}\|a-y^k\|_2^2 \right\} \\ y^{k+1} &= a^{k+1} \end{aligned}$$

or equivalently

$$a^{k+1} = \min_{a\in\tilde{A}} \left\{ J(a) + \frac{1}{2\lambda^k}\|a-a^k\|_2^2 \right\} \tag{6.5}$$

where λ^k is a sequence of positive numbers with $\lim_{k\to\infty}\lambda_k > 0$. An important part of the proximal point algorithm is solving the subproblem (6.5). The term

$$\frac{1}{2\lambda^k}\|a-a^k\|_2^2$$

is known as the regularization term and is strictly convex. This will guarantee that the subproblem has a unique minimizer for each k. We set

$$a^{k+1} = \min_{a\in\tilde{A}} \{ \mathscr{J}_P(a) \} \tag{6.6}$$

where

$$\mathscr{J}_P(a) = J(a) + \frac{1}{2\lambda^k}\|a-a^k\|_2^2 \tag{6.7}$$

The necessary and sufficient optimality condition for the above optimization problem is then the following variational inequality of finding $a^* \in \tilde{A}$:

$$\langle \nabla \mathscr{J}_P(a^*), a-a^* \rangle \geq 0 \ \ \forall a \in \tilde{A}. \tag{6.8}$$

In this chapter, we will look at the proximal point method described by Hager and Zhang [18]. Then using Kanzow [22]. We will incorporate different strategies to solve the subproblem and

combine them to method proposed by Hager and Zhang [18]. We will look at two more proximal point methods suggested by Han and Li. In each method, we will describe the algorithm, and test the method on four examples which are given on the next section. Some details on the proximal point methods are given in [2], [5], [19], [20], [23], [24], [32], [33], [34], [36], [50] and the cited differences therein.

6.2 Test Examples

We will test every method on the following four examples for each method:
Example 1.

$$\begin{aligned} f_1 &= 8\pi^2((2\pi^2(x^2+1)-1)\cos(2\pi x)+4\pi x\sin(2\pi x) \\ k_1 &= x^2+1 \\ z_1 &= \cos(2\pi x)-1. \end{aligned}$$

Example 2.

$$\begin{aligned} f_2 &= 4(90x^4-60x^3+42x^2-18x+13) \\ k_2 &= x^4+x^2+2 \\ z_2 &= x^2(x-1)^2. \end{aligned}$$

Example 3.

$$\begin{aligned} f_3 &= 32\pi^2(-631.65(x+0.4)(x^2-1.15x+0.6)\cos(4\pi x)-301.6(x-0.25)^2\sin(4\pi x)) \\ k_3 &= (2x-.5)^3+2 \\ z_3 &= \sin(4\pi x-0.5\pi)+1. \end{aligned}$$

Example 4.

$$\begin{aligned} f_4 &= 1764(x-0.773513)(x-0.5)(x-0.226487)(x^2-x+0.687621) \\ k_4 &= (x-0.5)^2+1 \\ z_4 &= x^2(x-1)^2(x-0.5)^3. \end{aligned}$$

6.3 Proximal-Like Methods Using Least Squares

The first method we use to solve the inverse problem was using the strategy suggested by Hager and Zhang. This involves the gradient of the proximal function, the gradient of the original function, and the difference between iterates. Proximal point method generates the iterative scheme by solving a minimization problem

$$a^{k+1} = \min_{a \in \tilde{A}} \mathscr{J}_P(a) \tag{6.9}$$

where

$$\mathscr{J}_P(a) = J(a) + \frac{1}{2}\mu_k \|a - a^k\|_2^2. \tag{6.10}$$

The subproblem is solved according to the following two criteria:

$$\mathscr{J}_P(a^{k+1}) \leq J(a^k) \tag{6.11a}$$

$$\|\nabla \mathscr{J}_P(a^{k+1})\| \leq \mu_k \|\nabla J(a^k)\|. \tag{6.11b}$$

This results in a fast convergence without using the Hessian of $J(a^k)$. Notice that in this scheme the least-square regularization term is used (cf. (6.10)). This strictly convex regularization term guarantees that the subproblem has a unique minimizer for each a. Hence this proximal point method is well-defined. The regularization parameter has the form

$$\mu^k = \beta \|\nabla J(a^k)\|^\eta,$$

where $\mu \in [0,2)$ and $\beta > 0$ is a constant to obtain convergence.

Algorithm 5.1

Initialization Step: Choose an initial guess a^0
Let $\mu_k = \beta \|\nabla J(a^k)\|^\eta$ and let $\gamma = 1$
Initialize β and η
Step 1: Find an a^{k+1} satisfying

$$\|\nabla \mathscr{J}_P(a^{k+1})\| \leq \mu_k \gamma \|\nabla J(a^k)\| \tag{6.12}$$

Step 2: If a^{k+1} satisfies

$$\mathscr{J}_P(a^{k+1}) \leq J(a^k) \tag{6.13}$$

Go to Step 3.

Else,

Set $\gamma = \gamma \times 0.1$ and go to Step 1,

End

Step 3: Let

$$a^k = a^{k+1}.$$

Step 4: Set $k = k+1$ and go to Step 1.

More specifically, in Step 1, the subproblem of (6.12) used a conjugate gradient method to find a^{k+1}.

In our experiments, we set

$$\mu_k = \beta \|\nabla J(a^k)\|^{\eta} = 0.5\|\nabla J(a^k)\|^1.$$

Example 1: Hager-Zhang Method using Least Squares

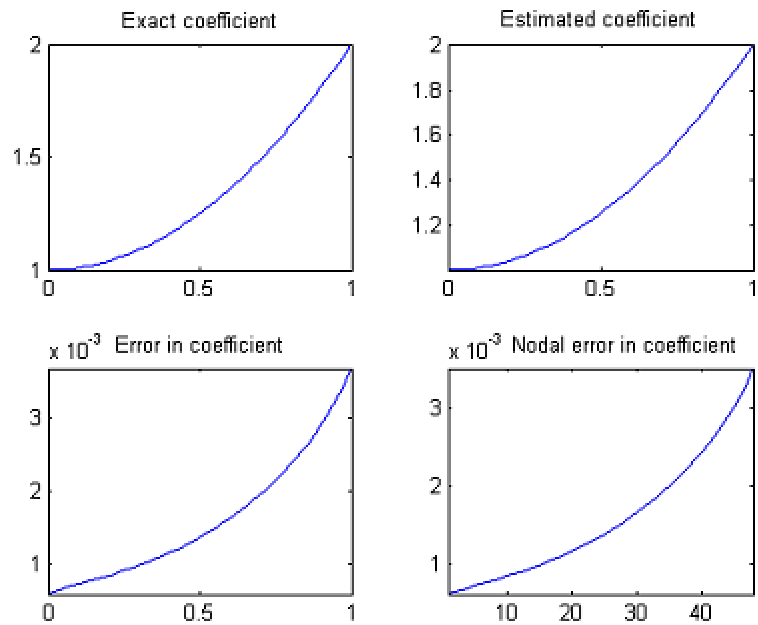


Figure 6.1: Example 1: Coefficient by Hager-Zhang Method using Least Squares

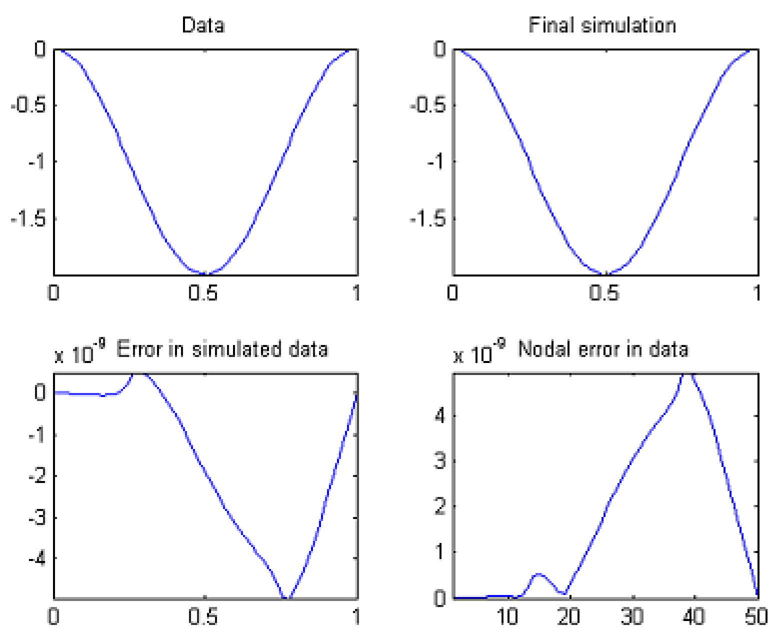


Figure 6.2: Example 1: Solution by Hager-Zhang Method using Least Squares

Example 2: Hager-Zhang Method using Least Squares

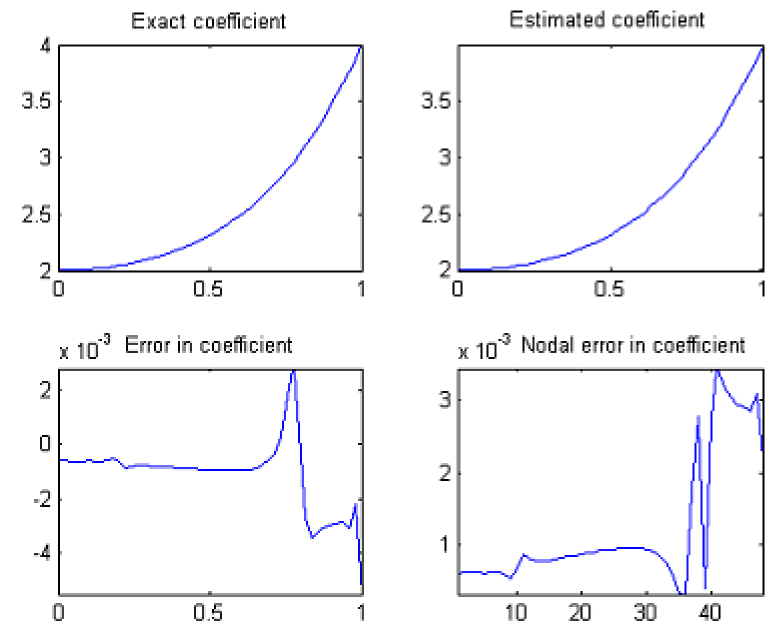


Figure 6.3: Example 2: Coefficient by Hager-Zhang Method using Least Squares

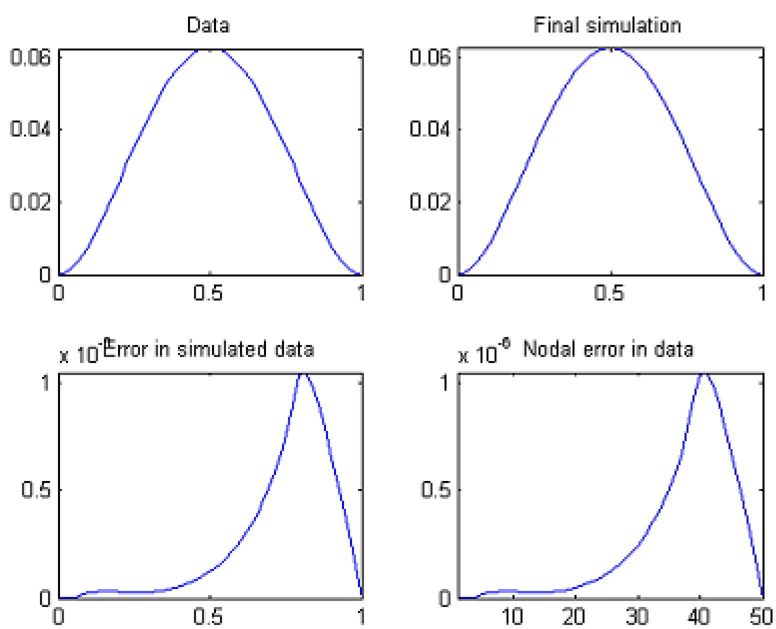


Figure 6.4: Example 2: Solution by Hager-Zhang Method using Least Squares

Example 3: Hager-Zhang Method using Least Squares

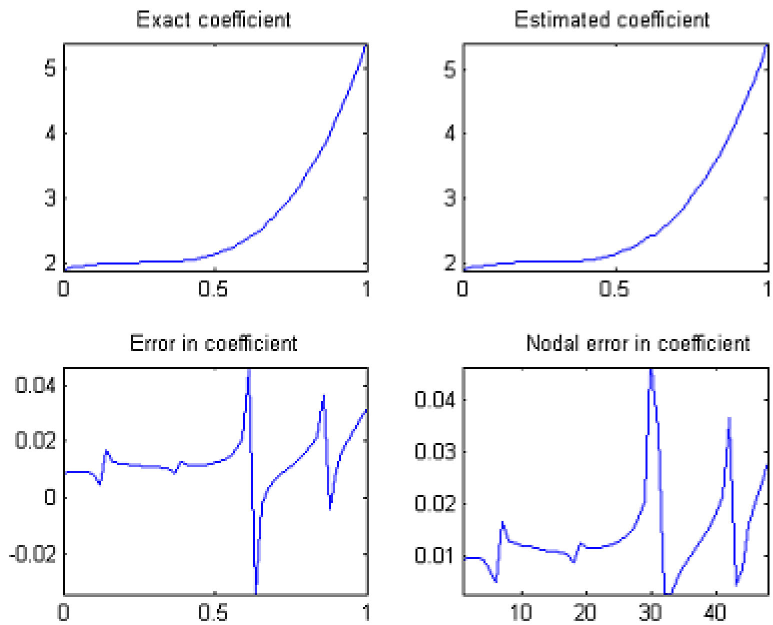


Figure 6.5: Example 3: Coefficient by Hager-Zhang Method using Least Squares

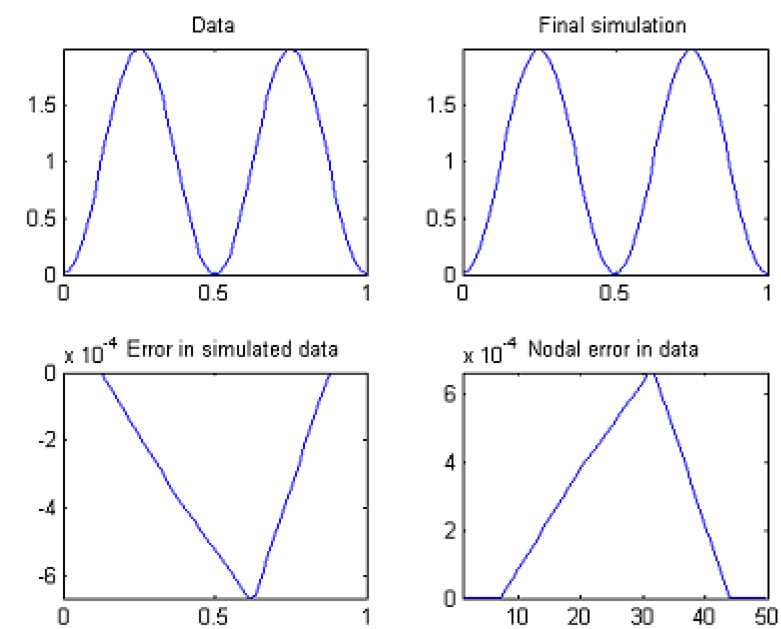


Figure 6.6: Example 3: Solution by Hager-Zhang Method using Least Squares

Example 4: Hager-Zhang Method using Least Squares

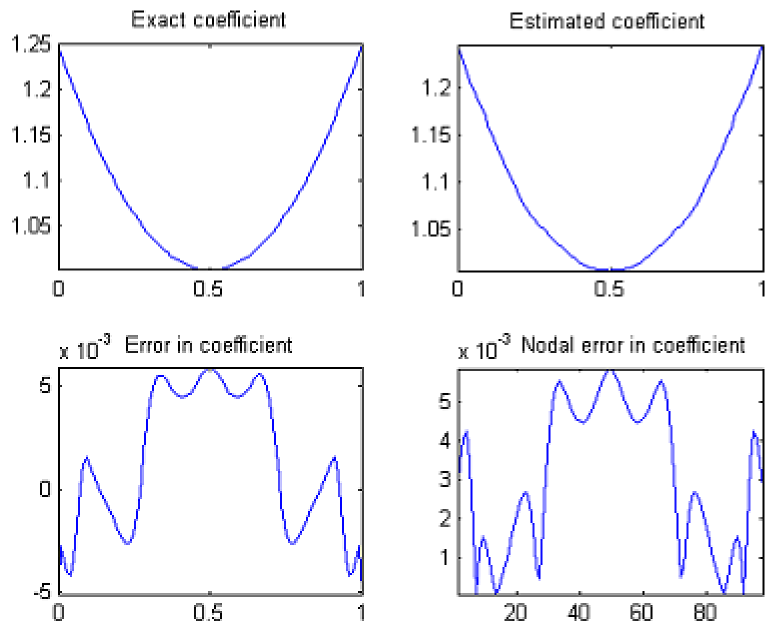


Figure 6.7: Example 4: Coefficient by Hager-Zhang Method using Least Squares

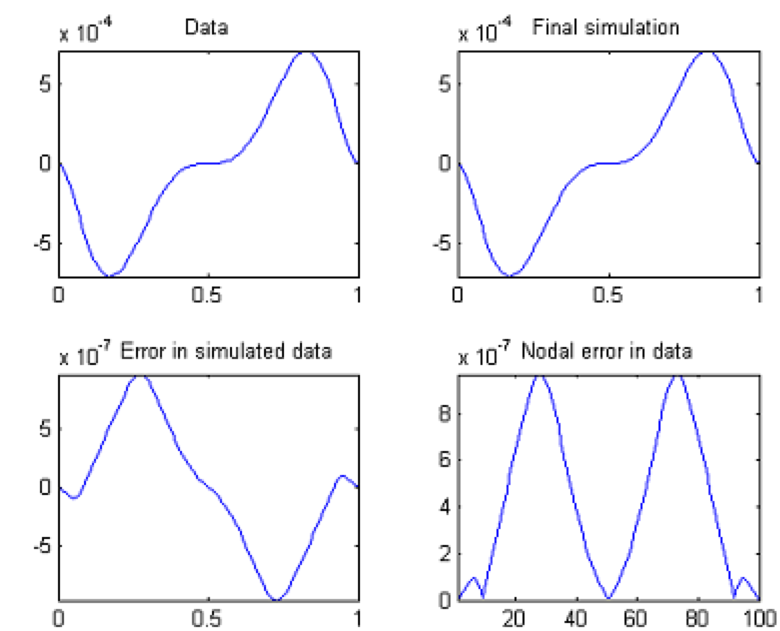


Figure 6.8: Example 4: Solution by Hager-Zhang Method using Least Squares

6.4 Proximal-like Methods Using φ-Divergence

This method is a variant of the classical proximal point method. Instead of using the strict convex quadratic term in the subproblem (6.7), this method uses φ-divergences functions to be the regularization term. In order to be a φ functions it must hold the following properties,

1. φ is twice continuously differentiable on $int(\Omega) = (0, +\infty)$.

2. φ is strictly convex on its domain.

3. $\lim_{t\to 0+} \dfrac{d\varphi(x)}{dx} = -\infty$.

4. $\varphi(1) = \frac{d\varphi(1)}{dx} = 0$ and $\frac{d^2\varphi(1)}{dx^2} > 0$.

5. There exists $v \in \left(\frac{1}{2}\frac{d^2\varphi(1)}{dx^2}, \frac{d^2\varphi(1)}{dx^2}\right)$ such that

$$\left(1 - \frac{1}{t}\right)\left(\frac{d^2\varphi(1)}{dx^2} + v(t-1)\right) \leq \frac{d\varphi(t)}{dx} \leq \frac{d^2\varphi(1)}{dx^2}(t-1) \quad \forall t > 0.$$

Instead of (6.6), the subproblem will be

$$a^{k+1} = \min\left\{\mathscr{J}_\varphi(a) \mid a \in \Omega\right\} \tag{6.14}$$

where

$$\mathscr{J}_\varphi(x) = J(a) + \mu_k d_\varphi(a, a^k) \tag{6.15}$$

and

$$d_\varphi(x,y) = \sum_{i=1}^{n} y_i \varphi\left(\frac{x_i}{y_i}\right). \tag{6.16}$$

A few examples of φ functions are,

$$\begin{aligned} \varphi_1(t) &= t\log t - t + 1 \\ \varphi_2(t) &= -\log t + t - 1 \\ \varphi_3(t) &= \left(\sqrt{t} - 1\right)^2. \end{aligned}$$

In our examples, we chose to use $\varphi_3(t)$ function and therefore the definition of d_φ is

$$d_\varphi(x,y) = \sum_{i=1}^{n} y_i \varphi\left(\sqrt{\frac{x_i}{y_i}} - 1\right)^2.$$

$$d_\varphi(a,a^k) = \sum_{i=1}^{n} a_i^k \varphi\left(\sqrt{\frac{a_i}{a_i^k}} - 1\right)^2,$$

and solving the subproblem

$$a^{k+1} = \min \left\{ J_2(a) + \mu_k \sum_{i=1}^{n} a_i^k \varphi \left(\sqrt{\frac{a_i}{a_i^k}} - 1 \right)^2 \quad \middle| \; a \in \Omega \right\}. \tag{6.17}$$

Algorithm 5.2

Initialization Step: Choose an initial x^0.
Let $\mu_k = \beta \|\nabla J(a^k)\|^\eta$ and let $\gamma = 1$
Initialize β and η
Step 1: Find an a^{k+1} satisfying

$$\|\nabla \mathscr{J}_\varphi(a^{k+1})\| \leq \mu_k \gamma \|\nabla J(a^k)\| \tag{6.18}$$

Step 2: If a^{k+1} satisfies

$$\mathscr{J}_\varphi(a^{k+1}) \leq J(a^k) \tag{6.19}$$

Go to Step 3.
Else,
Set $\gamma = \gamma \times 0.1$ and go to step 1,
End
Step 3: Let

$$a^k = a^{k+1}.$$

Step 4: Set $k = k+1$ and go to step 1.

More specifically, in Step 1, the subproblem of (6.18) used a conjugate gradient method to find a^{k+1}.
In our experiments, we set $\mu_k = \beta \|\nabla J(a^k)\|^\eta = 0.5\|\nabla J(a^k)\|^1$.

Example 1: Hager-Zhang Method using φ-divergence

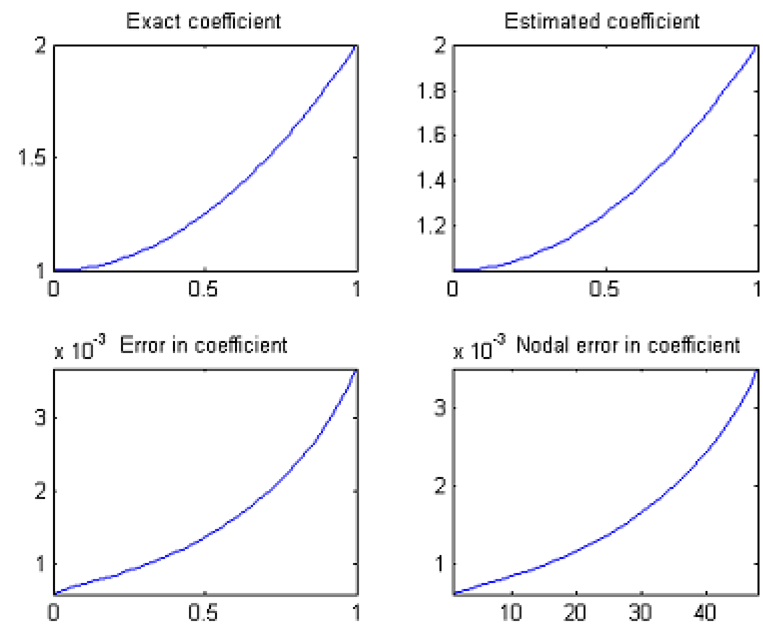


Figure 6.9: Example 1: Coefficient by Hager-Zhang Method using φ-divergence

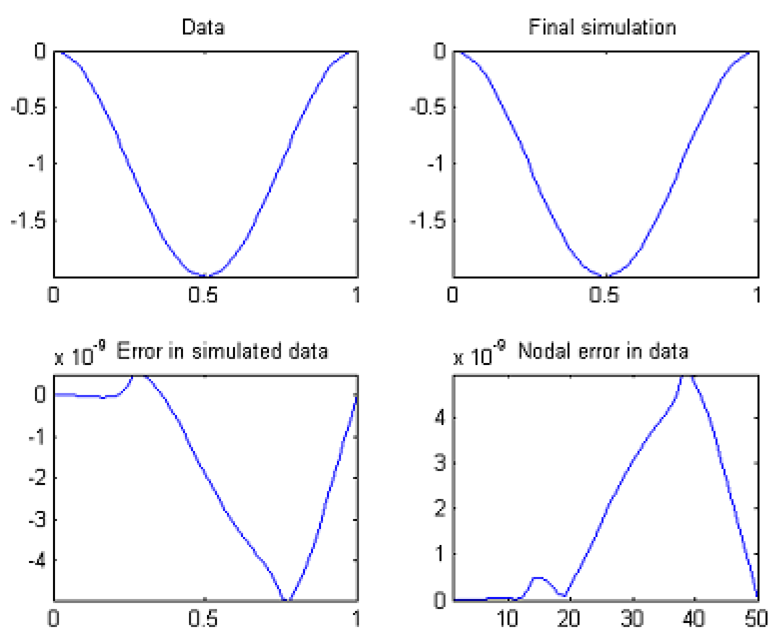


Figure 6.10: Example 1: Solution by Hager-Zhang Method using φ-divergence

Example 2: Hager-Zhang Method using φ-divergence

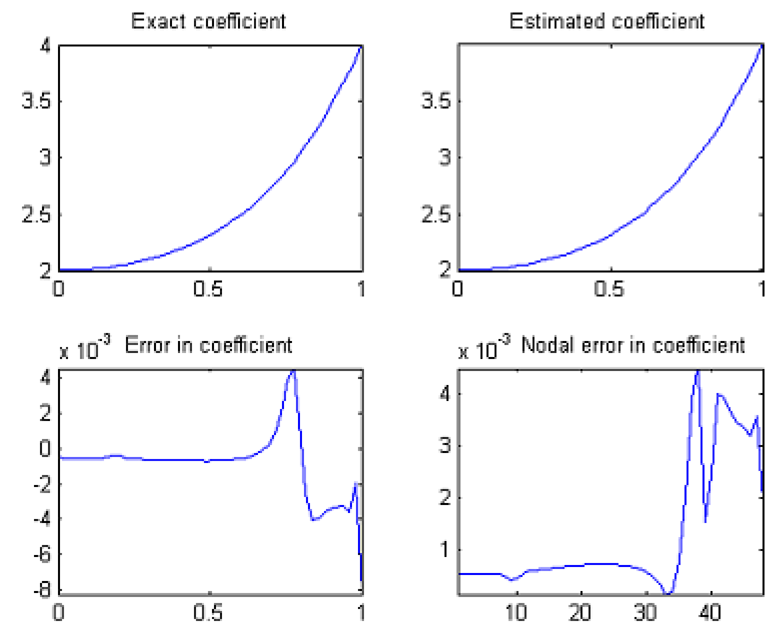


Figure 6.11: Example 2: Coefficient by Hager-Zhang Method using φ-divergence

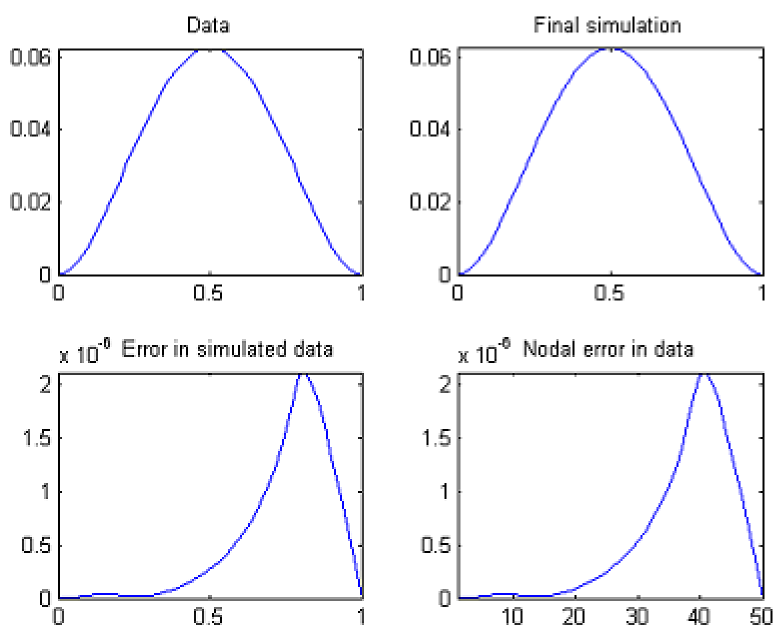


Figure 6.12: Example 2: Solution by Hager-Zhang Method using φ-divergence

Example 3: Hager-Zhang Method using φ-divergence

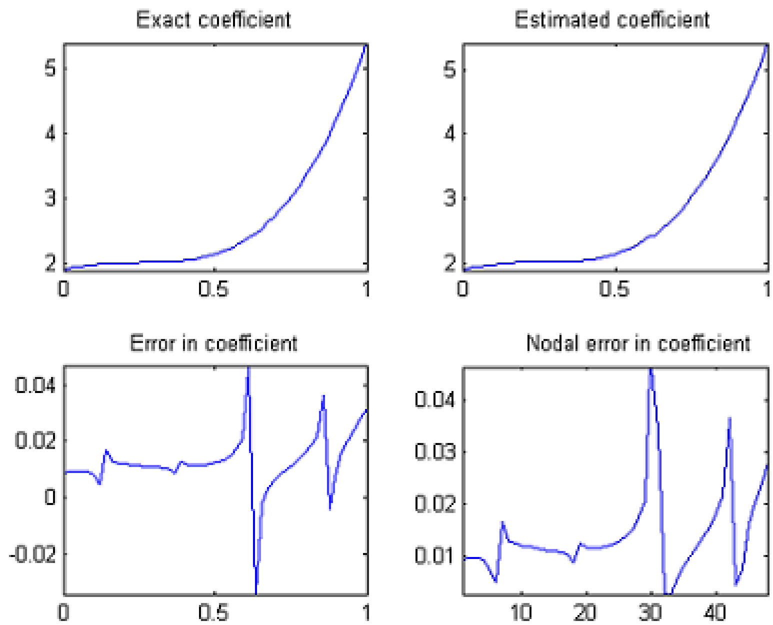


Figure 6.13: Example 3: Coefficient by Hager-Zhang Method using φ-divergence

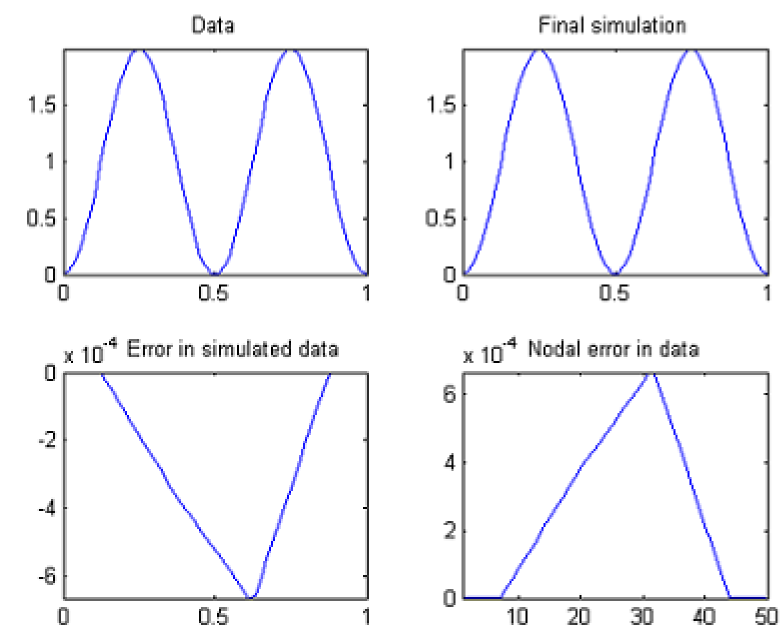


Figure 6.14: Example 3: Solution by Hager-Zhang Method using φ-divergence

Example 4: Hager-Zhang Method using φ-divergence

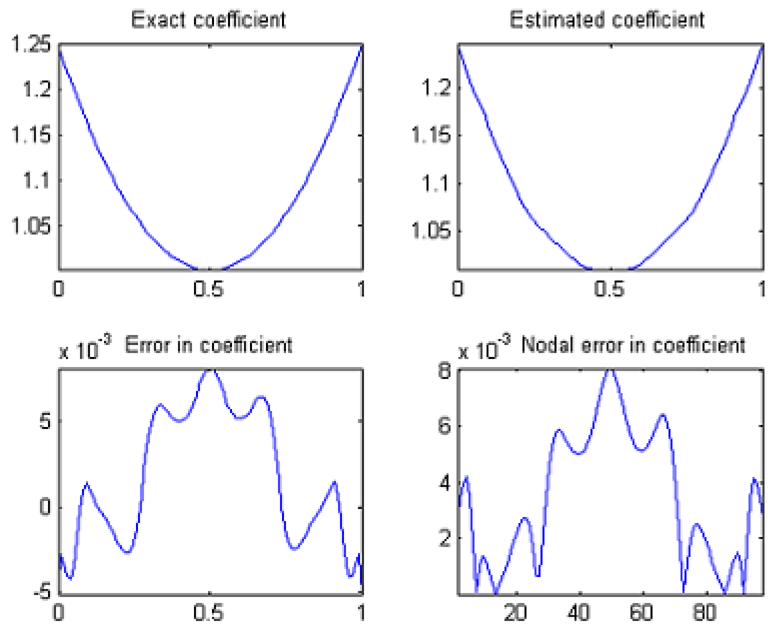


Figure 6.15: Example 4: Coefficient by Hager-Zhang Method using φ-divergence

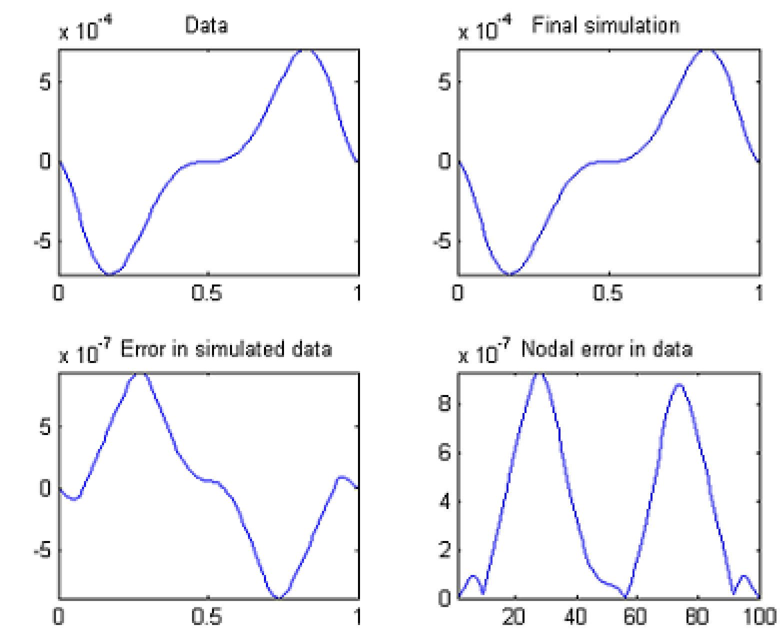


Figure 6.16: Example 4: Solution by Hager-Zhang Method using φ-divergence

6.5 Proximal-like Methods Using Bregman Functions

This method uses Bregman functions which are more general convex functions. It involves replacing the least squares or φ-divergence term by another strictly convex function

$$D_\psi(x,y) = \psi(x) - \psi(y) - \nabla\psi(y)^T(x-y), \tag{6.20}$$

where ψ is the so-called Bregman function.
Let S be an open and convex set and a mapping $\psi : \bar{S} \to \mathbb{R}$. In order to be a Bregman function, it must hold the following properties:

1. ψ is strictly convex and continuous on $\bar{S}$.

2. ψ is continuously differentiable in S.

3. The partial level set
$$L_\alpha = \{y \in \bar{S} | D_\psi(x,y) \leq \alpha\}$$
is bounded for every $x \in \bar{S}$.

4. If $\{y^k\} \subset S$ converges to x, then $\lim\limits_{k\to\infty} D_\psi(x,y^k) = 0$.

Instead of (6.6), the subproblem will be

$$a^{k+1} = \min\left\{\mathscr{J}_\psi(a) \mid a \in \Omega\right\}, \tag{6.21}$$

where

$$\mathscr{J}_\psi(x) = J(a) + \mu_k D_\psi(a,a^k) \tag{6.22}$$

and

$$D_\psi(x,y) = \psi(x) - \psi(y) - \nabla\psi(y)^T(x-y). \tag{6.23}$$

A few examples of Bregman functions are,

$$\begin{aligned}
\psi_1(x) &= \frac{1}{2}\|x\|^2 \\
\psi_2(x) &= \sum_{i=1}^{n} x_i \log x_i - x_i \\
\psi_3(x) &= -\sum_{i=1}^{n} \log x_i,
\end{aligned}$$

and there respective convex-like functions

$$\begin{aligned} D_1(x,y) &= \frac{1}{2}\|x-y\|^2 \\ D_2(x,y) &= \sum_{i=1}^{n} x_i \log\frac{x_i}{y_i} + y_i - x_i \\ D_3(x,y) &= -\sum_{i=1}^{n} \frac{x_i}{y_i} - \log\frac{x_i}{y_i} - 1. \end{aligned}$$

In our problem, we know the coefficient must be within a lower and upper limit otherwise known as a box constraints, $0 < l_i < a_i < u_i < \infty$. A Bregman function that satisfies the box constraints and the one that we use our example is,

$$\psi_4(a^k) = \sum_{i=1}^{n} (a_i - l_i)\log(a_i - l_i) + (u_i - a_i)\log(u_i - a_i^k) \tag{6.24}$$

$$D_4(a^k, y) = \sum_{i=1}^{n} (a_i - l_i)\log\left(\frac{a_i - l_i}{a_i^k - l_i}\right) + (u_i - a_i)\log\left(\frac{u_i - a_i}{u_i - a_i^k}\right). \tag{6.25}$$

We are solving the subproblem

$$a^{k+1} = \min\left\{ J_2(a) + \mu_k \sum_{i=1}^{n} (a_i - l_i)\log\left(\frac{a_i - l_i)}{a_i^k - l_i}\right) + (u_i - a_i)\log\left(\frac{u_i - a_i)}{u_i - a_i^k}\right) \;\middle|\; a \in \Omega \right\}.$$

Algorithm 5.3

Initialization Step: Choose an initial a^0. Let $\mu_k = \beta\|\nabla J(a^k)\|^{\eta}$ and let $\gamma = 1$. Initialize β and η. **Step 1.** Find an a^{k+1} satisfying

$$\|\nabla \mathscr{J}_{\psi}(a^{k+1})\| \le \mu_k \gamma \|\nabla J_2(a^k)\| \tag{6.26}$$

Step 2. If a^{k+1} satisfies

$$\mathscr{J}_{\psi}(a^{k+1}) \le J(a^k) \tag{6.27}$$

Go to Step 3.

Else,

Set $\gamma = \gamma \times 0.1$ and go to Step 1,

End

Step 3. Let

$$a^k = a^{k+1}.$$

Step 4. Set $k = k+1$ and go to Step 1.

More specifically, in Step 1, the subproblem of (6.26) used a conjugate gradient method to find a^{k+1}

In our experiments, we set $\mu_k = \beta\|\nabla J(a^k)\|^\eta = 0.5\|\nabla J(a^k)\|^1$.

Example 1: Hager-Zhang Method using Bregman Function

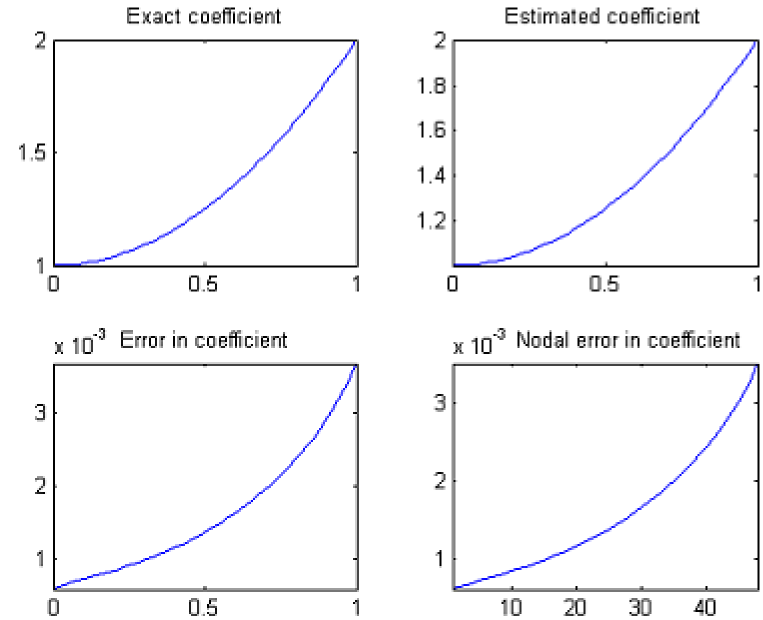


Figure 6.17: Example 1: Coefficient by Hager-Zhang Method using Bregman function

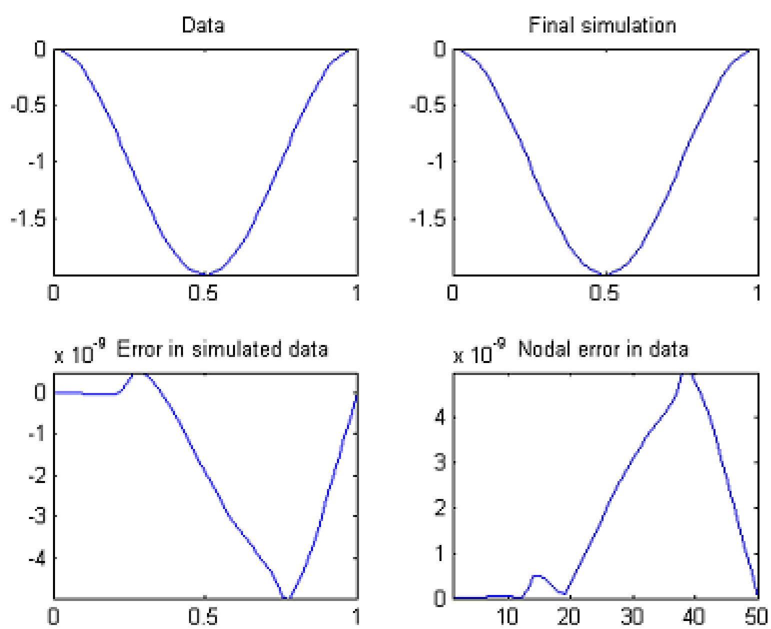


Figure 6.18: Example 1: Solution by Hager-Zhang Method using Bregman function

Example 2: Hager-Zhang Method using Bregman Function

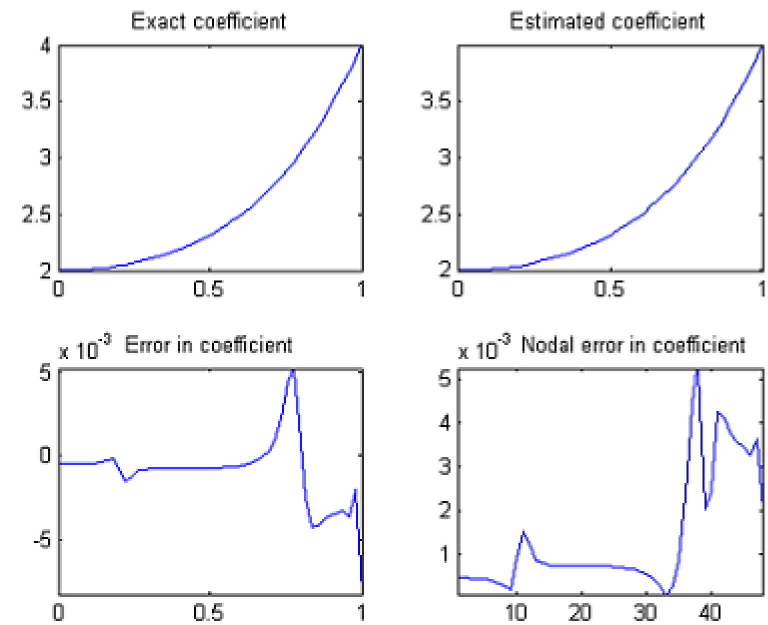


Figure 6.19: Example 2: Coefficient by Hager-Zhang Method using Bregman function

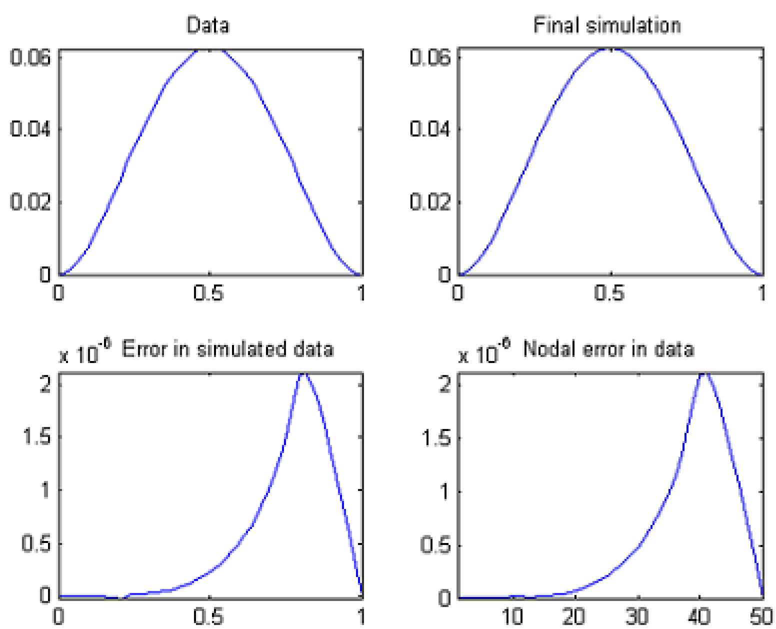


Figure 6.20: Example 2: Solution by Hager-Zhang Method using Bregman function

Example 3: Hager-Zhang Method using Bregman Function

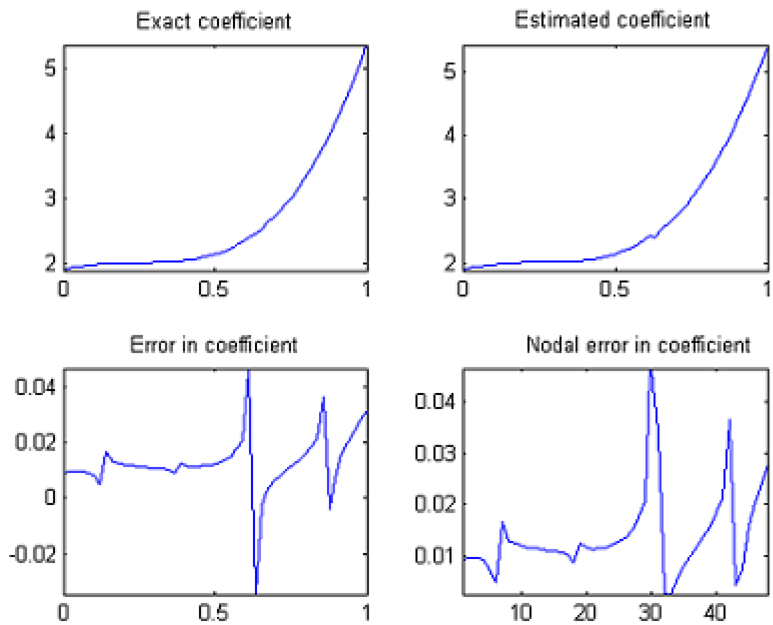


Figure 6.21: Example 3: Coefficient by Hager-Zhang Method using Bregman function

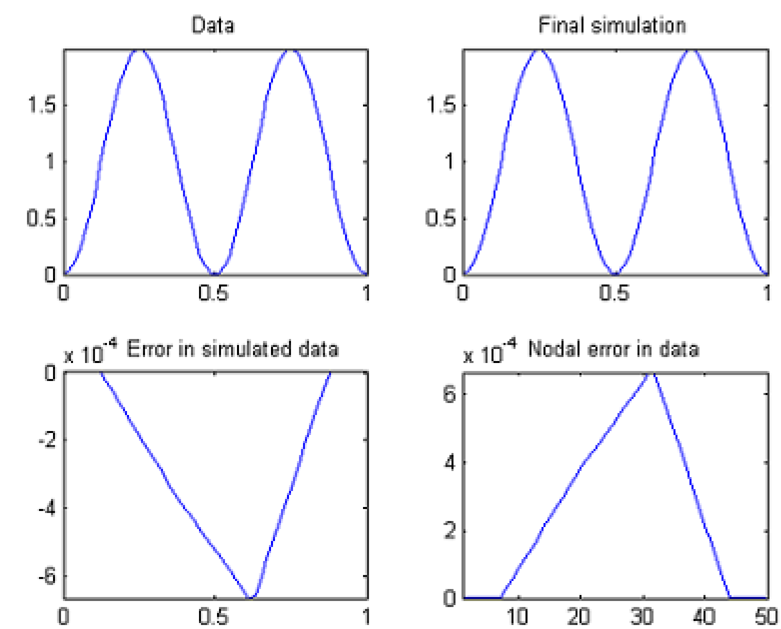


Figure 6.22: Example 3: Solution by Hager-Zhang Method using Bregman function

Example 4: Hager-Zhang Method using Bregman Function

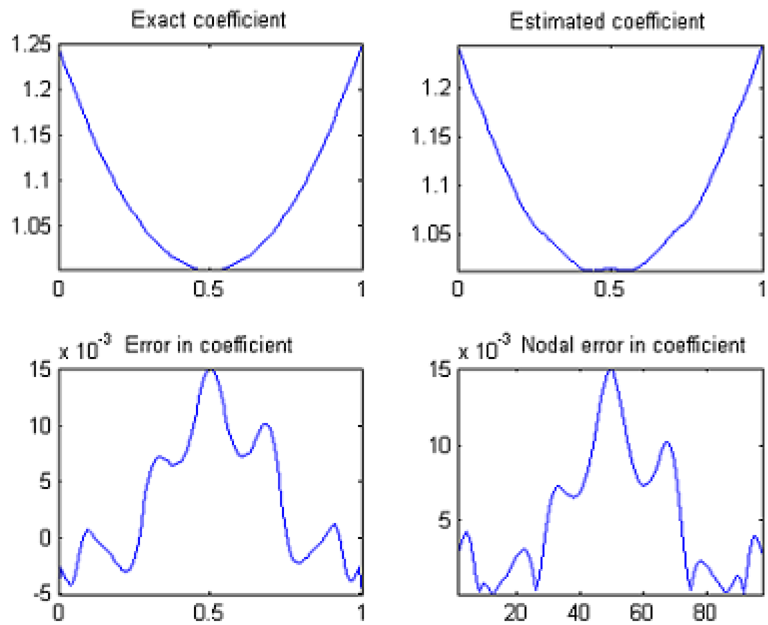


Figure 6.23: Example 4: Coefficient by Hager-Zhang Method using Bregman function

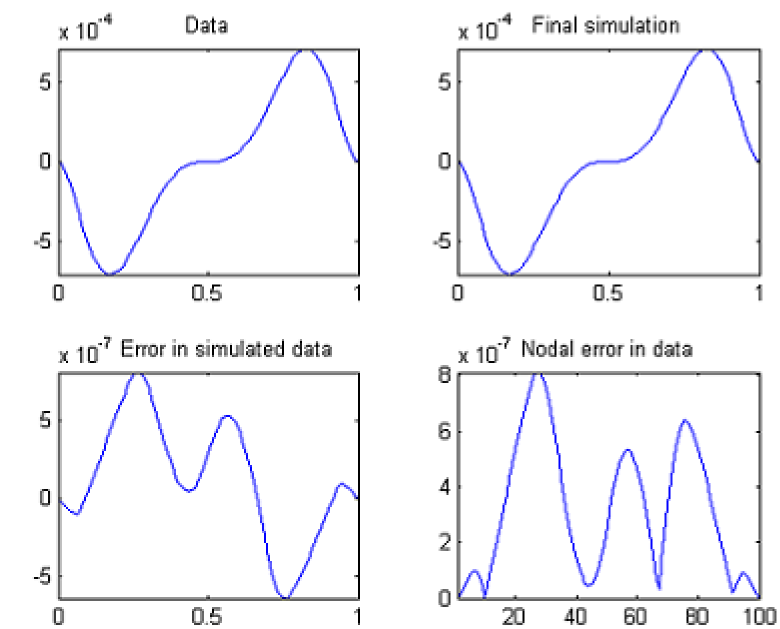


Figure 6.24: Example 4: Solution by Hager-Zhang Method using Bregman function

6.6 Proximal-like Methods Using Modified φ-Divergence

In the φ-divergence method, we used a conjugate gradient method to solve the subproblem. Now we would like to solve the subproblem by using Newton's method. This method involves knowing the second order derivative and the Hessian matrix of the objective functional. With φ-divergence, we have (6.32)

$$d_\varphi(x,y) = \sum_{i=1}^{n} y_i \varphi\left(\frac{x_i}{y_i}\right).$$

The second derivative of this gives us

$$\nabla^2_{xx} d_\varphi(x,y) = \sum_{i=1}^{n} \frac{1}{y_i} \frac{d^2\varphi}{dx^2}\left(\frac{x_i}{y_i}\right) e_i e_i^T,$$

where e_i is the ith unit vector.

This is a problem since the factor $\frac{1}{y_i}$ goes to infinity during the iteration process for all indices for which a constraint like $x_i \geq 0$ is a solution. This will lead to an ill-condition Hessian matrix. To avoid this, the modification comes by replacing the y_i term in the φ function to y_i^2. Then the factor of $\frac{1}{y_i}$ will not exist in the second derivative. Now the modified φ-divergence function can be represented by

$$\bar{d}_\varphi(x,y) = \sum_{i=1}^{n} y_i^2 \varphi\left(\frac{x_i}{y_i}\right), \tag{6.28}$$

and the second derivative by

$$\nabla^2_{xx} \bar{d}_\varphi(x,y) = \sum_{i=1}^{n} \frac{1}{y_i} \frac{d^2\varphi}{dx^2}\left(\frac{x_i}{y_i}\right) e_i e_i^T. \tag{6.29}$$

Instead of (6.6), the subproblem will be

$$a^{k+1} = \min\left\{ \bar{\mathscr{J}}_\varphi(a) \mid a \in \Omega \right\} \tag{6.30}$$

where

$$\bar{\mathscr{J}}_\varphi(x) = J(a) + \frac{1}{\lambda^k} \bar{d}_\varphi(a, a^k) \tag{6.31}$$

and

$$\bar{d}_\varphi(x,y) = \sum_{i=1}^{n} y_i \varphi\left(\frac{x_i}{y_i}\right). \tag{6.32}$$

In our examples, we chose to use $\varphi_3(t) = \left(\sqrt{t}-1\right)^2$ function and therefore the definition of $\bar{d}_\varphi$ is

$$\bar{d}_\varphi(x,y) = \sum_{i=1}^{n} y_i^2 \varphi\left(\sqrt{\frac{x_i}{y_i}}-1\right)^2.$$

$$\bar{d}_\varphi(a,a^k) = \sum_{i=1}^{n} (a_i^k)^2 \varphi\left(\sqrt{\frac{a_i}{a_i^k}}-1\right)^2,$$

and solving the subproblem

$$a^{k+1} = \min\left\{ J_2(a) + \frac{1}{\lambda^k}\sum_{i=1}^{n}(a_i^k)^2\varphi\left(\sqrt{\frac{a_i}{a_i^k}}-1\right)^2 \quad \middle| \; a \in \Omega \right\}$$

Algorithm 5.4

Initialization: Choose an initial a^0.
Let $\mu_k = \beta\|\nabla J(a^k)\|^\eta$ and let $\gamma = 1$.
Initialize β and η
Step 1. Find an a^{k+1} satisfying

$$\|\nabla \bar{\mathscr{J}}_\varphi(a^{k+1})\| \le \mu_k \gamma \|\nabla J(a^k)\|. \tag{6.33}$$

Step 2. If a^{k+1} satisfies

$$\bar{\mathscr{J}}_\varphi(a^{k+1}) \le J(a^k) \tag{6.34}$$

Go to Step 3.
Else,
Set $\gamma = \gamma \times 0.1$ and go to step 1,
End
Step 3. Let

$$a^k = a^{k+1}.$$

Step 4. Set $k = k+1$ and go to step 1.
More specifically, in Step 1, the subproblem of (6.33) used a conjugate gradient method to find a^{k+1}. In our experiments, we set $\mu_k = \beta\|\nabla J(a^k)\|^\eta = 0.5\|\nabla J(a^k)\|^1$

Example 1: Hager-Zhang Method using Quadratic function

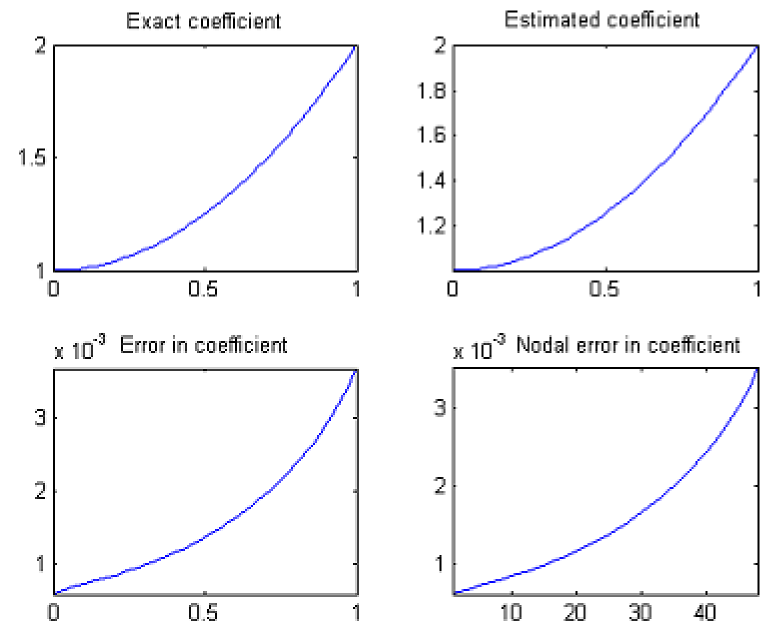


Figure 6.25: Example 1: Coefficient by Hager-Zhang Method using quadratic function

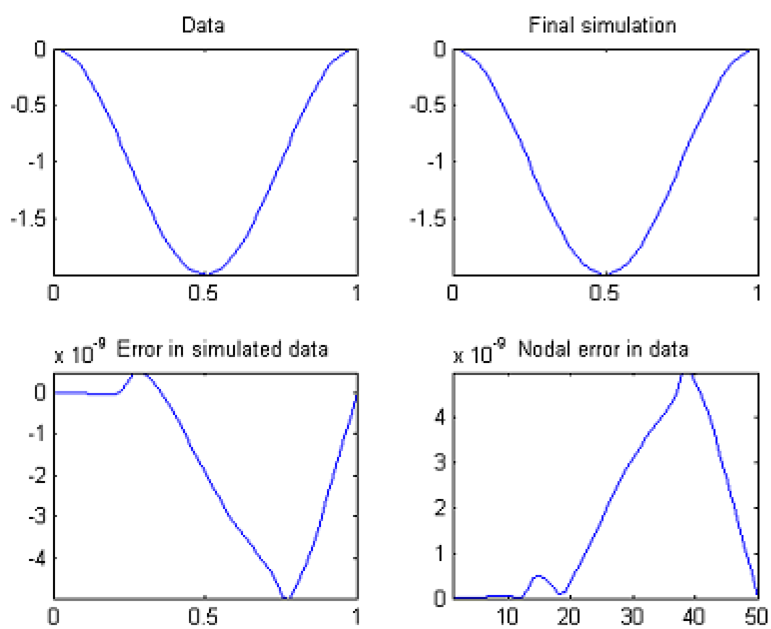


Figure 6.26: Example 1: Solution by Hager-Zhang Method using quadratic function

Example 2: Hager-Zhang Method using Quadratic function

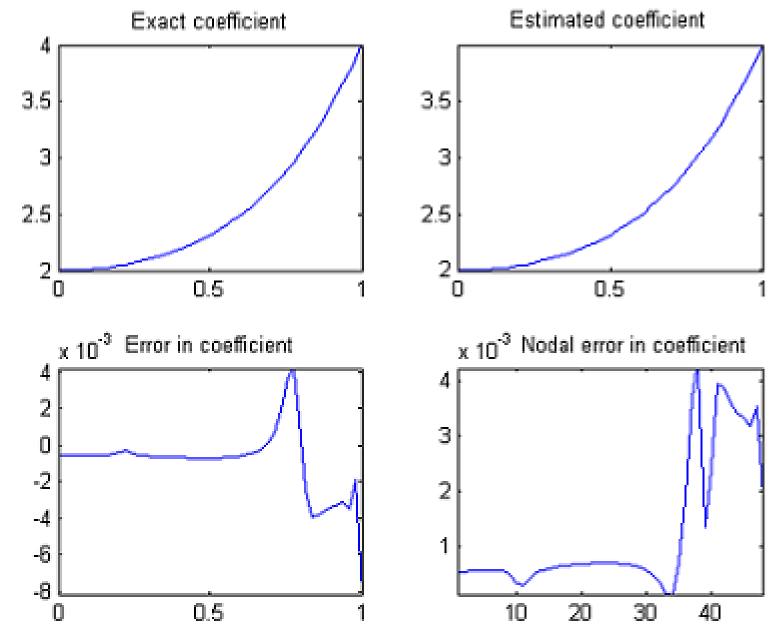


Figure 6.27: Example 2: Coefficient by Hager-Zhang Method using quadratic function

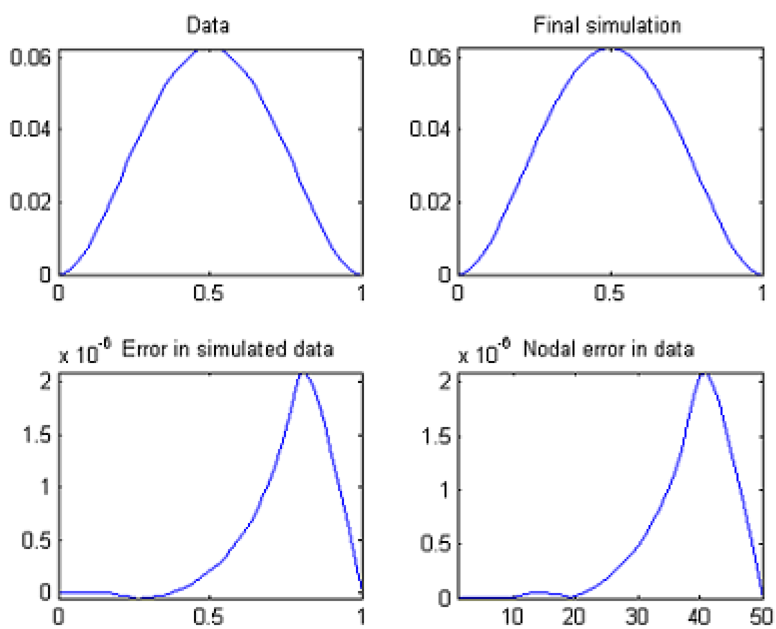


Figure 6.28: Example 2: Solution by Hager-Zhang Method using quadratic function

Example 3: Hager-Zhang Method using Quadratic function

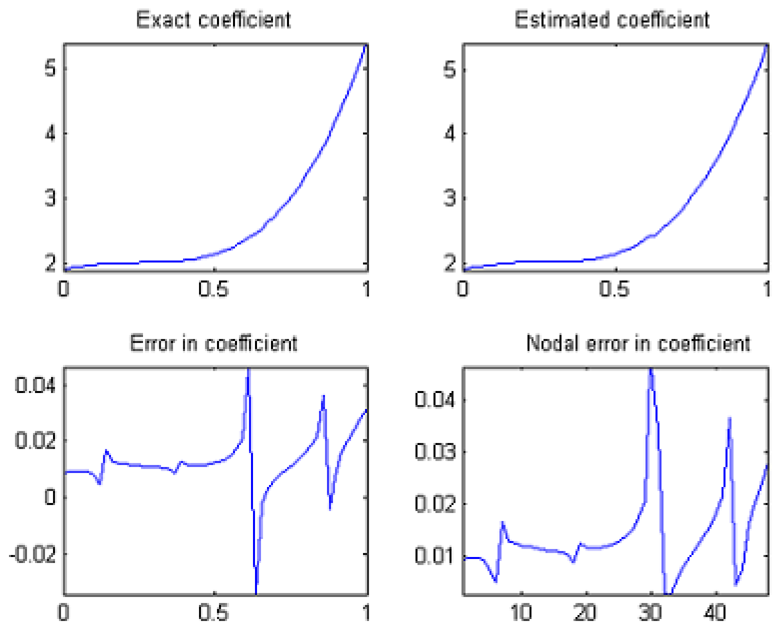


Figure 6.29: Example 3: Coefficient by Hager-Zhang Method using quadratic function

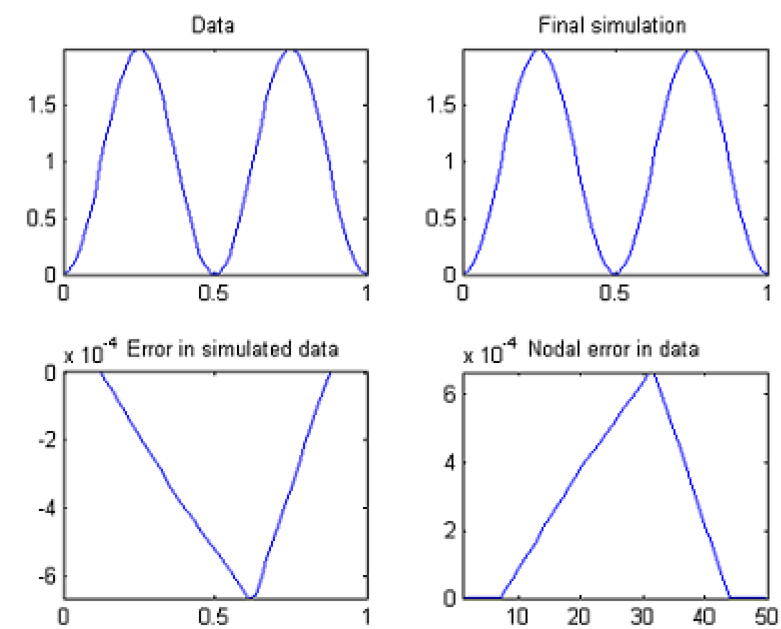


Figure 6.30: Example 3: Solution by Hager-Zhang Method using quadratic function

Example 4: Hager-Zhang Method using Quadratic function

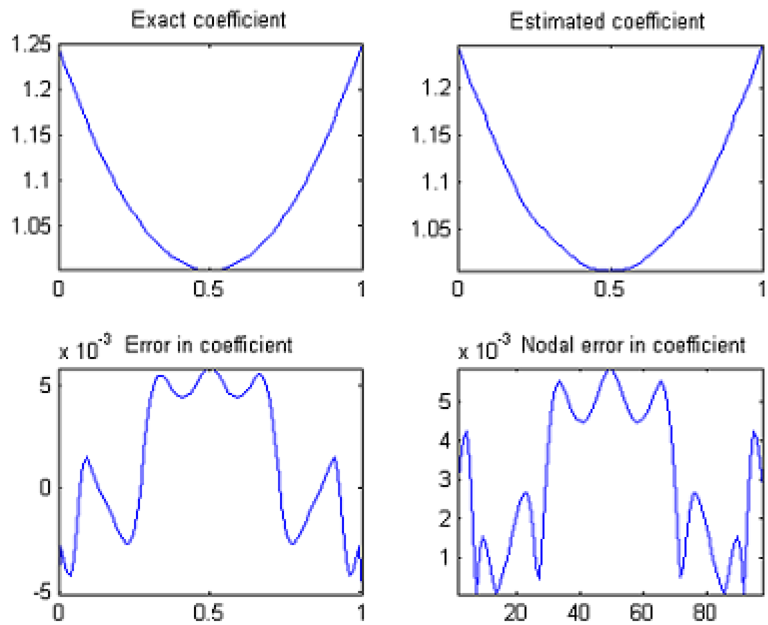


Figure 6.31: Example 4: Coefficient by Hager-Zhang Method using quadratic function

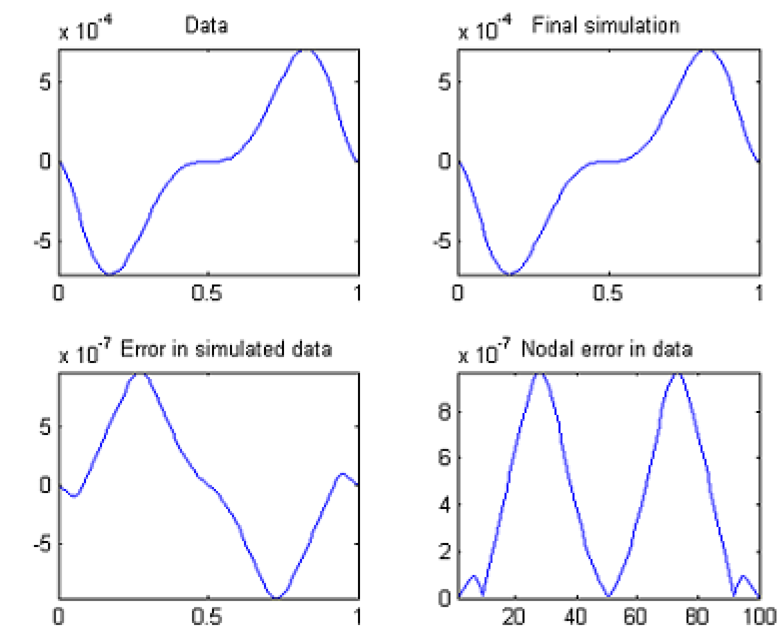


Figure 6.32: Example 4: Solution by Hager-Zhang Method using quadratic function

6.7 Han Proximal-Point Method

This method features a Bregman function-based proximal point algorithm for solving the variational inequality problem. The first method we adapted for the inverse problem was using the stopping criteria from Hager-Zhang. Recall that the two criteria are

$$\mathscr{J}_P(a^{k+1}) \leq J(a^k) \quad (6.35a)$$

$$\|\nabla \mathscr{J}_P(a^{k+1})\| \leq \mu_k \|\nabla J(a^k)\|. \quad (6.35b)$$

Algorithm 5.5

Initialization Step: Choose an appropriate Bregman function.
Choose an initial a^0
Initialize $\sigma \in (0,1)$ and $0 < c_k < \infty$
Step 1. Find an y^k satisfying

$$\|r^k\| \leq \sigma \|a^k - y^k\| \quad (6.36)$$

where

$$\|r^k\| = c_k(\nabla J_P(y^k) + \nabla h(y^k) - \nabla h(a^k)) + (y^k - a^k)$$

Step 2. Compute a^{k+1},

$$a^{k+1} = (1-t)\mathrm{Proj}[a^k - c_k \alpha_k \nabla J_P(y^k)] + t a^k \quad (6.37)$$

where

$$\alpha_k = \frac{\langle \nabla J_P(y^k), a^k - y^k \rangle}{c_k \|\nabla J(y^k)\|^2}$$

Step 3. Set $k = k+1$ and go to Step 1.
More specifically, in Step 1, the subproblem of (6.36) used a Newton method to find a^{k+1}.
In our experiments, we set $c_k = \frac{1}{\|\nabla(a^k)\|}$.

Example 1: Han Method

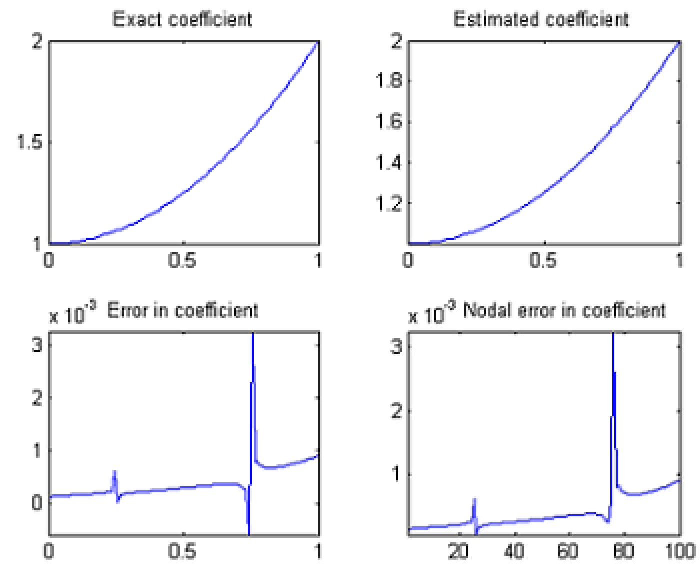


Figure 6.33: Example 1: Coefficient by Han Method

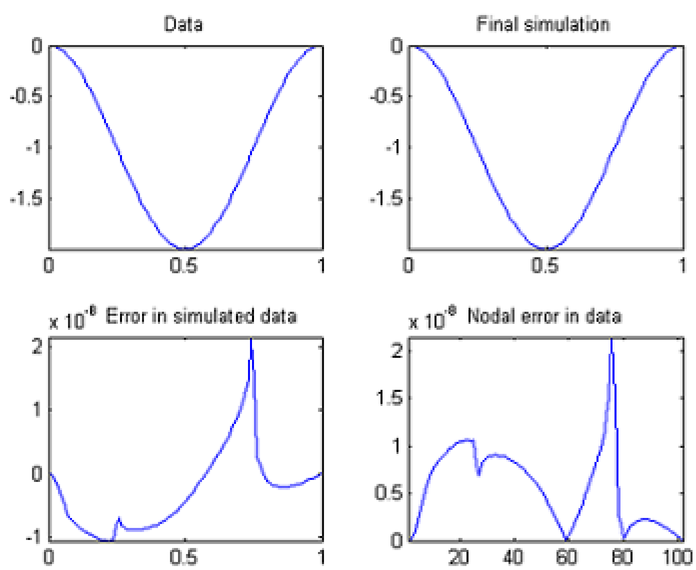


Figure 6.34: Example 1: Solution by Han Method

Example 2: Han Method

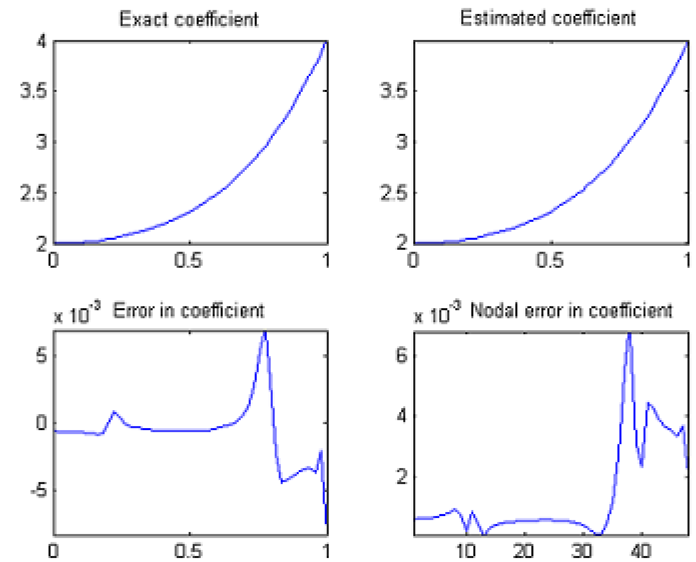


Figure 6.35: Example 2: Coefficient by Han Method

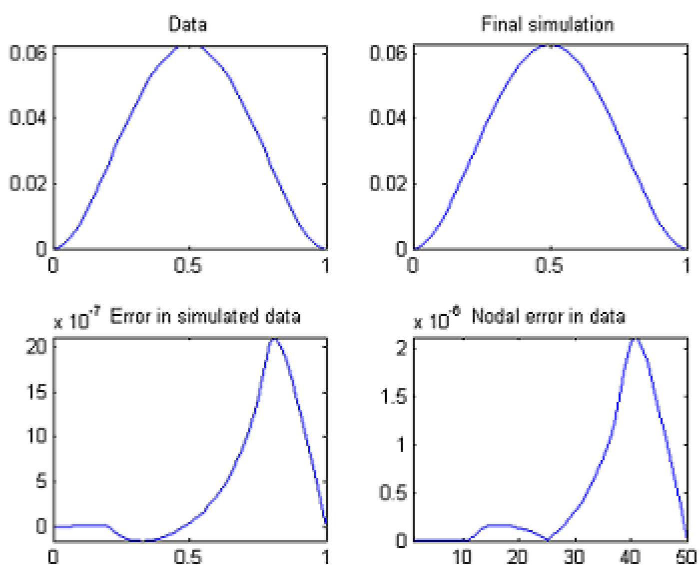


Figure 6.36: Example 2: Solution by Han Method

Example 3: Han Method

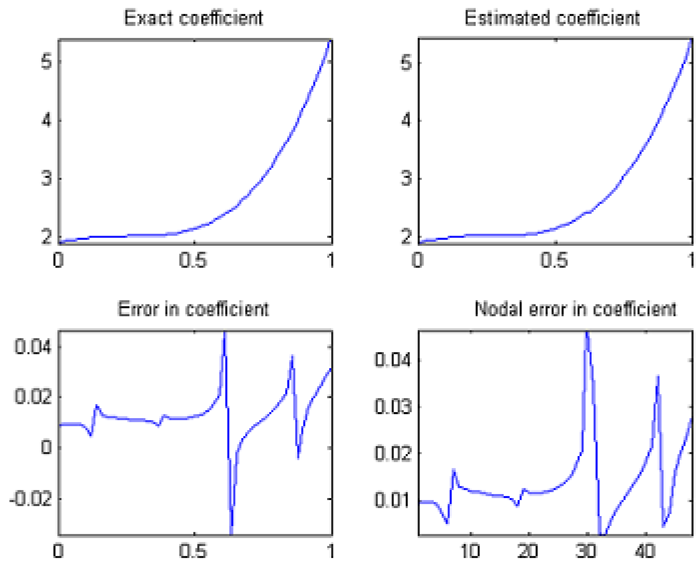


Figure 6.37: Example 3: Coefficient by Han Method

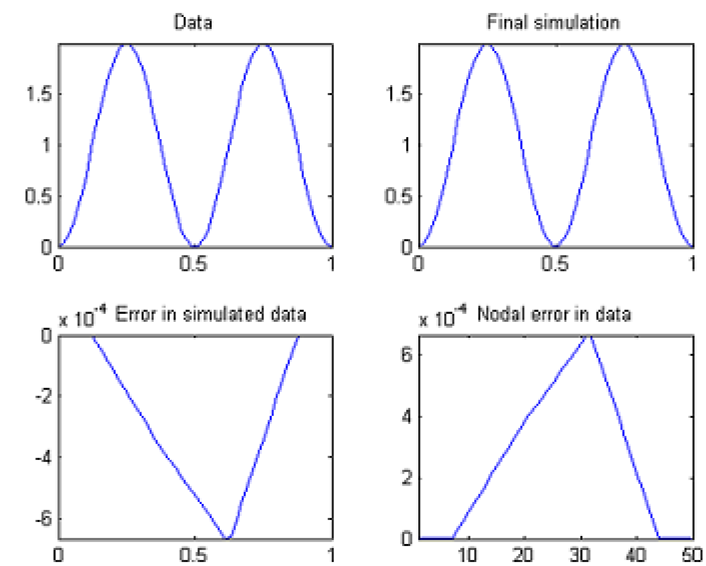


Figure 6.38: Example 3: Solution by Han Method

Example 4: Han Method

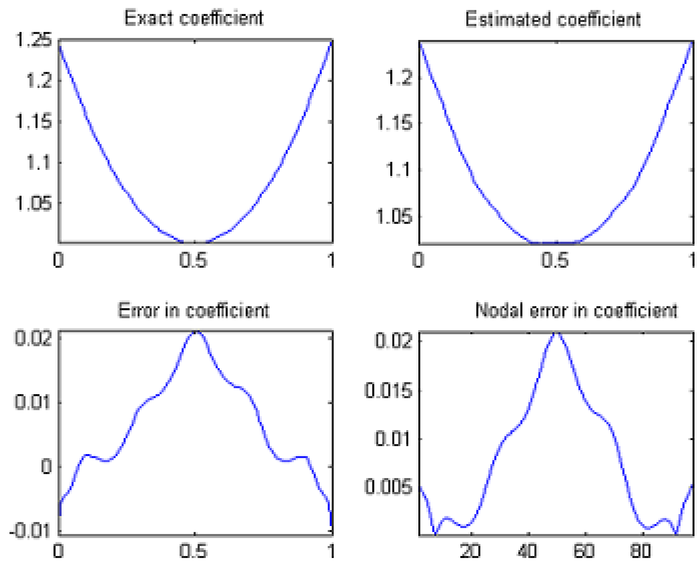


Figure 6.39: Example 4: Coefficient by Han Method

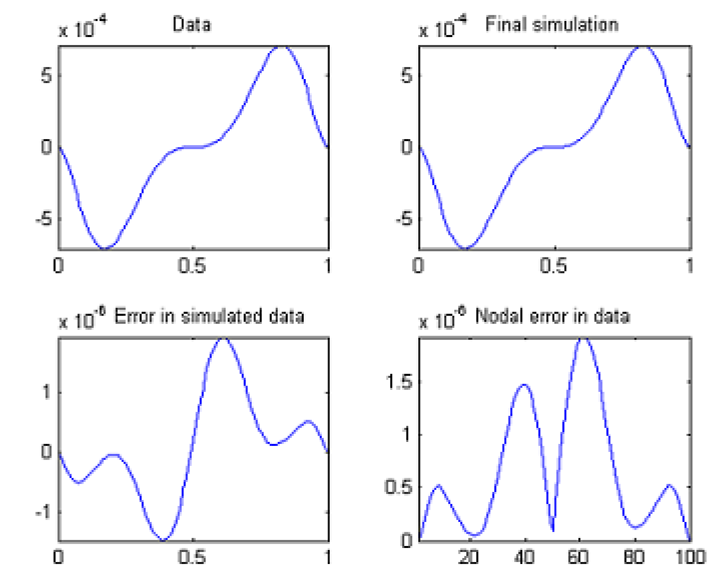


Figure 6.40: Example 4: Solution by Han Method

6.8 Li-Yuan Proximal Point Method

The next method we employ is by Li and Yuan. Their aim was to make better adjustments on the subproblem and to optimize the step-size in the gradient step.

Algorithm 5.6

Initialization Step. Choose an initial a^0
Initialize $\sigma \in (0,1)$, $v \in (0,1)$, and $1 < \gamma_k < 2$. **Step 1.** Find an y^k satisfying

$$\Delta(y^k) \le v(\|a^k - y^k\|^2 + \|a^k - y^k\|) \tag{6.38}$$

where

$$\begin{aligned} \Delta(y^k) &= \langle 2(y^k - \tilde{y}^k), \nabla J(y^k)\rangle - \|y^k - \tilde{y}^k\|^2 \\ \tilde{y}^k &= \mathrm{Proj}[a^k - \lambda_k \nabla J(y^k)] \end{aligned}$$

Step 2. Correct the approximation y^k,

$$\tilde{a}^k = \mathrm{Proj}[a^k - \alpha_k \lambda_k \nabla J_P(y^k)] \tag{6.39}$$

where

$$\alpha_k = \frac{\|a^k - \tilde{a}^k\|^2 - \langle \lambda_k (y^k - \tilde{y}^k), \nabla J_P(yk)\rangle}{\|a^k - \tilde{y}^k\|^2}$$

Step 3. Compute a^{k+1},

$$a^{k+1} = \mathrm{Proj}[a^k - \gamma_k \tau_k (a^k - \tilde{a}^k)] \tag{6.40}$$

where

$$\tau_k = 1 + \frac{\langle \alpha_k \lambda_k (\tilde{a}^k - y^k), \nabla J_P(y^k)\rangle}{\|a^k - \tilde{a}^k\|^2}$$

Step 4. Set $k = k+1$ and go to Step 1.

More specifically, in Step 1, the subproblem of (6.38) used a Newton method to find a^{k+1}.

Example 1: Li-Yuan Method

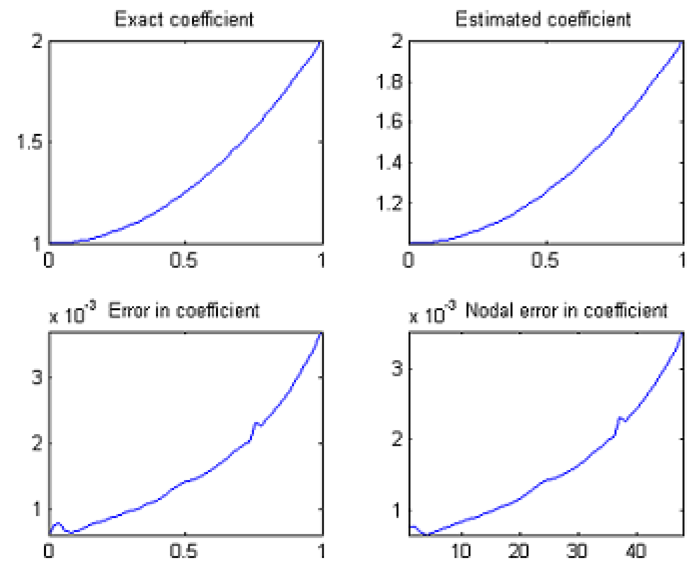


Figure 6.41: Example 1: Coefficient by Li-Yuan Method

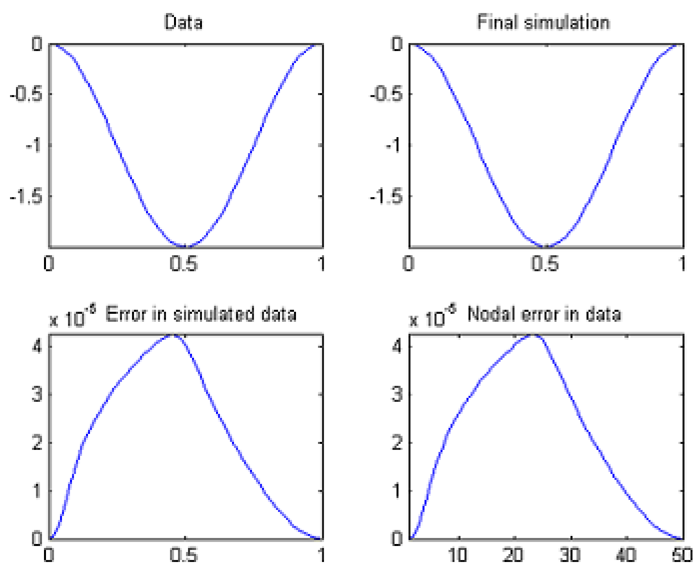


Figure 6.42: Example 1: Solution by Li-Yuan Method

Example 2: Li Method

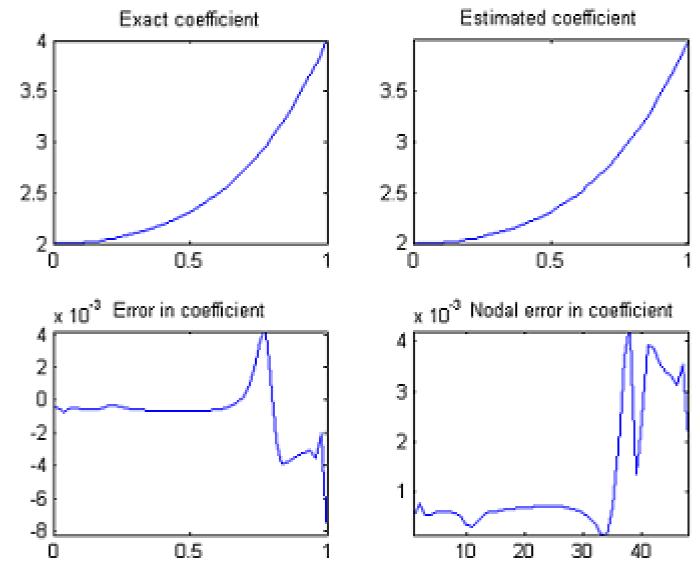


Figure 6.43: Example 2: Coefficient by Li-Yuan Method

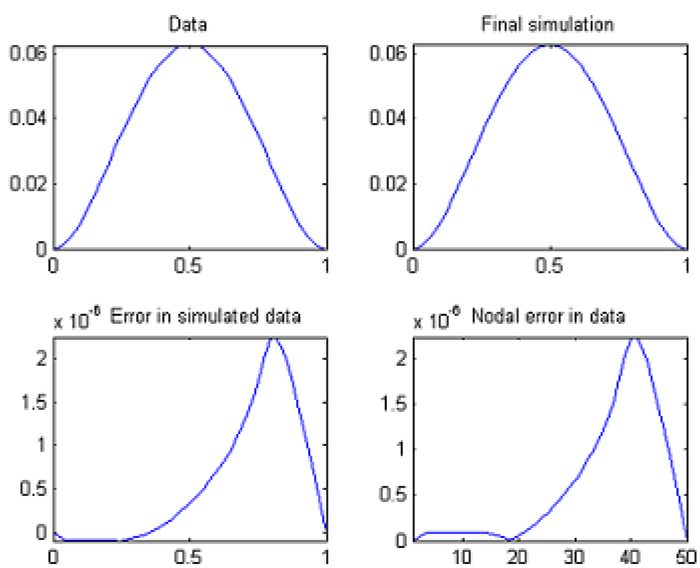


Figure 6.44: Example 2: Solution by Li-Yuan Method

Example 3: Li-Yuan Method

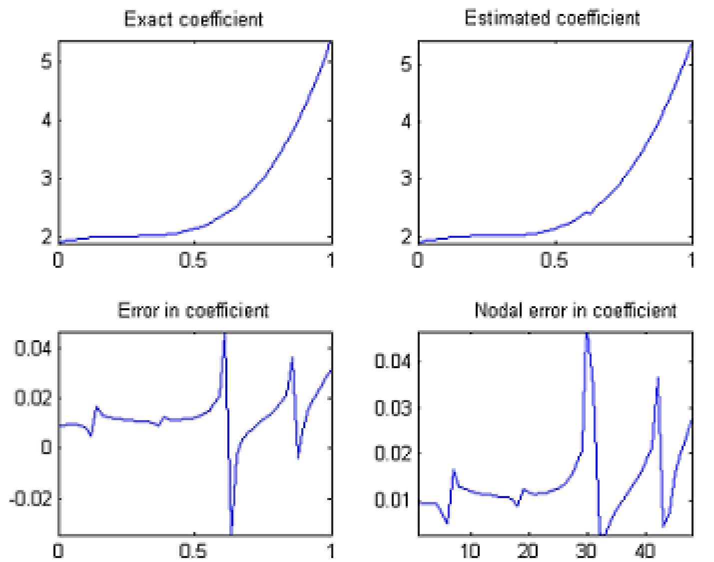


Figure 6.45: Example 3: Coefficient by Li-Yuan Method

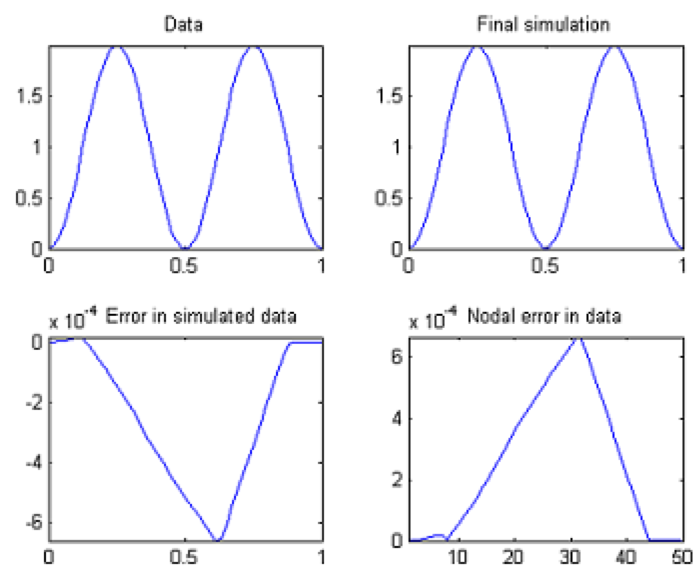


Figure 6.46: Example 3: Solution by Li-Yuan Method

Example 4: Li-Yuan Method

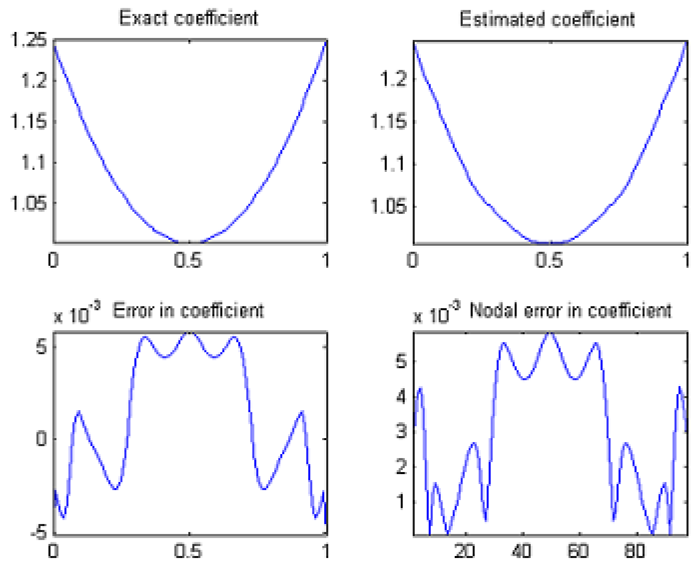


Figure 6.47: Example 4: Coefficient by Li Method

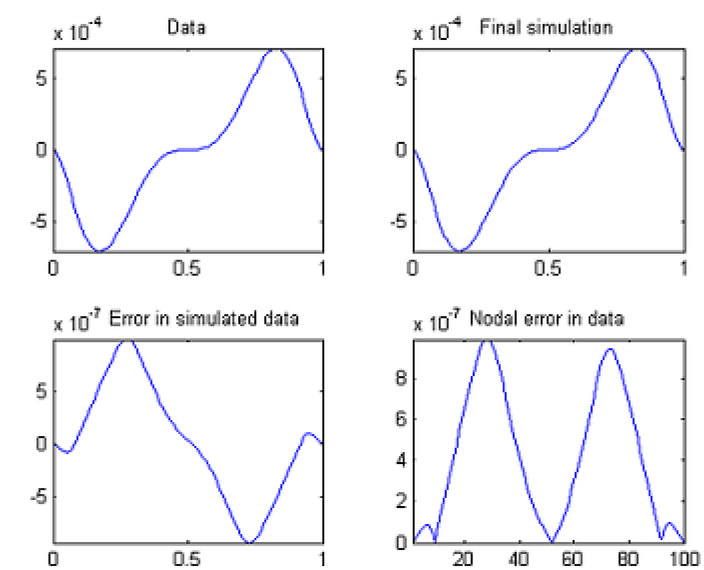


Figure 6.48: Example 4: Solution by Li-Yuan Method

Chapter 7

Comparative Performance Analysis

In this chapter we compare the various proximal point algorithms that we have employed in this work.

7.1 Numerical Results for Example 1

We would like to compare the results of Hager and Zhang's proximal point algorithm. We make this discussion in terms of Example 1. Table 7.1 contains the results for this example. Each of Hager and Zhang's first derivative each have roughly the same numbers, while Hager and Zhang's quadratic has the best performance as far as time is concerned. Recall that Hager and Zhang's quadratic Method uses the Newton method to solve the subproblem, unlike the conjugate gradient method. In each of Hager and Zhang's method, we set $\beta = 0.05$, and $\mu = 1$. Then testing the method on many epsilon's from $1e-1, 5e-2, 1e-2, 5e-3, 1e-3, ..., 1e-10$. The best results occurred when epsilon=$1e-6$, and $N = 50$.
In the following, let LS stand for the method involving Least Squares, let φ stand for the method involving φ-divergence, and the other two of Hanger and Zhang's method be the Bregman function, and the quadratic method.
We want to look at two parameters, the number of functions evaluation, and the time to complete the computation. In general, Hager and Zhang's proximal point method gives very good results, being computed in a very reasonable time. The proximal point method of Han's, and Li and Yuan's lack in the number of functions and on time. However the stopping criteria of the subproblem were different for Han, and Li and Yaun. We are more interested in the algorithms proposed by Hager and Zhang. In each of Hager and Zhang's method the initial value of β was

set to 0.05 and Hager-Zhang note that β should be a sufficiently small. In his numerical results, he uses $\beta = 0.05$, which is what lead me to use it for my own numerical results. Since Hager and Zhang don't specify exactly what β is, we wanted to explore this a bit more. We then ran each of Hager and Zhang's method for example one with the β value ranging from 0.01 to 0.1 by steps of 0.01 and the results are shown in tables 7.2 to table 7.5.

It is important to note that Hager and Zhang-quadratic method can only be used when the Hessian form is available for use. If it is not available the best first derivative method would be Hager and Zhang- φ, but either of the other two will work just as good.

We rearrange table 7.1 by using the best β values from each method in table **??** Now we are able to see that the already reasonably good results are now even better. Notice the time's are all roughly the same with Hager-Zhang quadratic method still being a bit better in time, but also now the number of function's evaluated are much better. All the methods showed much better results when β values were lower than 0.05 (the original initial value).

Other examples experience the same performance of proximal point methods and hence we only give the tables containing the numerical results.

Method	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
Hager and Zhang-LS	865	783	NA	5	2.2138
Hager and Zhang-φ	869	792	NA	5	2.2394
Hager and Zhang-Bregman	856	775	NA	5	2.2044
Hager and Zhang-Quadratic	3609	3496	85	5	0.7286
Han	181844	179171	1739	127	29.9905
Li and Yuan	5122	3852	NA	1270	29.9202

Table 7.1: Results of Example 1.

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	521	496	NA	3	1.3721
0.02	909	831	NA	4	2.3844
0.03	864	797	NA	5	2.2442
0.04	888	809	NA	5	2.2990
0.05	865	783	NA	5	2.2601
0.06	851	782	NA	5	2.1912
0.07	897	814	NA	5	2.3321
0.08	620	590	NA	4	1.9805
0.09	926	850	NA	5	2.3916
0.10	839	774	NA	4	2.4310

Table 7.2: Example 1. Using Hager and Zhang-LS

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	591	563	NA	3	1.5696
0.02	525	500	NA	3	1.4301
0.03	504	480	NA	4	1.3420
0.04	812	744	NA	5	2.1116
0.05	869	792	NA	5	2.2390
0.06	826	747	NA	5	2.1499
0.07	843	763	NA	5	2.18530
0.08	844	777	NA	4	2.2062
0.09	811	746	NA	4	2.1657
0.10	784	714	NA	4	2.0441

Table 7.3: Example 1. Using Hager and Zhang-φ

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	591	563	NA	3	1.5738
0.02	939	852	NA	4	2.4800
0.03	921	847	NA	5	2.4224
0.04	894	817	NA	5	2.3555
0.05	856	775	NA	5	2.2461
0.06	810	745	NA	5	2.1094
0.07	879	799	NA	5	2.3223
0.08	778	741	NA	4	2.0573
0.09	666	634	NA	4	1.7689
0.10	688	655	NA	4	1.8227

Table 7.4: Example 1. Using Hager and Zhang-Bregman Function

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	4040	3934	77	3	0.7290
0.02	479	466	9	3	0.1476
0.03	430	417	8	4	0.1595
0.04	431	417	8	4	0.1923
0.05	4307	4193	82	5	0.7452
0.06	4256	4142	81	5	0.7388
0.07	4308	4193	82	5	0.9739
0.08	538	520	10	4	0.2139
0.09	538	520	10	4	0.1845
0.10	538	520	10	4	0.1891

Table 7.5: Example 1 Using Hager and Zhang-Quadratic Function

Method	β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
Hager and Zhang-LS	0.01	521	496	NA	3	1.3721
Hager and Zhang-φ	0.03	504	480	NA	4	1.3420
Hager and Zhang-Breg	0.01	591	563	NA	3	1.5739
Hager and Zhang-Quad	0.03	430	417	8	4	0.1595

Table 7.6: New Results of Example 1.

7.2 Numerical Results for Example 2

Method	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
Hager and Zhang-NR	157	146	NA	2	0.4800
Hager and Zhang-LS	323	205	NA	4	0.9358
Hager and Zhang-φ	276	154	NA	3	0.8297
Hager and Zhang-Bregman	284	153	NA	3	0.8421
Hager and Zhang-Quadratic	4282	4140	81	4	0.8565
Han	66839	64859	1271	20	17.5445
Li and Yuan	2028	1597	NA	432	11.4972

Table 7.7: Results of Example 2.

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	67	64	NA	1	0.2237
0.02	67	62	NA	1	0.2249
0.03	67	62	NA	1	0.2260
0.04	157	146	NA	2	0.4731
0.05	157	146	NA	2	0.4710
0.06	141	131	NA	2	0.4190
0.07	141	131	NA	2	0.4202
0.08	141	131	NA	2	0.4251
0.09	141	131	NA	2	0.4280
0.10	141	131	NA	2	0.4182

Table 7.8: Example 2. Using Hager and Zhang-NR

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	241	153	NA	3	0.6960
0.02	274	191	NA	3	0.8317
0.03	259	191	NA	3	0.7582
0.04	367	249	NA	4	1.0540
0.05	323	205	NA	4	0.9552
0.06	361	229	NA	4	1.0626
0.07	310	185	NA	4	1.0313
0.08	346	232	NA	4	1.0185
0.09	345	203	NA	4	1.0135
0.10	317	207	NA	4	0.9097

Table 7.9: Example 2. Using Hager and Zhang-LS

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	211	110	NA	2	0.5789
0.02	284	145	NA	2	0.8319
0.03	123	86	NA	2	0.3443
0.04	170	100	NA	2	0.4905
0.05	276	154	NA	3	0.8264
0.06	223	119	NA	3	0.6589
0.07	290	156	NA	3	0.8716
0.08	186	116	NA	3	0.5654
0.09	222	128	NA	3	0.6604
0.10	284	159	NA	3	0.8317

Table 7.10: Example 2. Using Hager and Zhang-φ

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	228	107	NA	2	0.6300
0.02	244	129	NA	2	0.7546
0.03	272	139	NA	3	0.7686
0.04	229	123	NA	3	0.6872
0.05	284	153	NA	3	0.8595
0.06	268	146	NA	3	0.8018
0.07	278	148	NA	3	0.8166
0.08	243	136	NA	3	0.7295
0.09	264	140	NA	3	0.7802
0.10	276	147	NA	3	0.8131

Table 7.11: Example 2. Using Hager and Zhang-Bregman Function

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	3451	3322	65	2	0.7665
0.02	3195	3067	60	2	0.7287
0.03	767	721	14	3	0.3272
0.04	2279	2149	42	3	0.6296
0.05	4282	4140	81	4	0.8793
0.06	883	825	16	4	0.3217
0.07	830	774	15	4	0.3223
0.08	3107	2967	58	4	0.7920
0.09	2698	2559	50	4	0.7106
0.10	2545	2406	47	4	0.9290

Table 7.12: Example 2. Using Hager and Zhang-Quadratic Function

Method	β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
Hager and Zhang-NR	0.02	67	64	NA	1	0.2249
Hager and Zhang-LS	0.01	241	153	NA	3	0.6960
Hager and Zhang-φ	0.03	123	86	NA	2	0.3443
Hager and Zhang-Breg	0.01	228	107	NA	2	0.6300
Hager and Zhang-Quad	0.03	767	721	14	3	0.3272

Table 7.13: New Results of Example Two

7.3 Numerical Results for Example 3

Method	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
Hager and Zhang-NR	348	295	NA	5	0.8531
Hager and Zhang-LS	361	300	NA	6	0.8809
Hager and Zhang-φ	324	282	NA	6	0.9049
Hager and Zhang-Bregman	280	267	NA	5	0.7294
Hager and Zhang-Quadratic	4458	4351	85	6	0.7085
Han	64538	62360	1222	22	19.1101
Li and Yuan	4989	3831	NA	1136	27.2631

Table 7.14: Results of Example 3.

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	351	298	NA	6	0.8701
0.02	352	299	NA	7	0.8981
0.03	347	294	NA	5	0.8730
0.04	349	296	NA	6	0.8752
0.05	348	295	NA	5	0.8720
0.06	348	295	NA	5	0.8940
0.07	351	298	NA	6	0.9015
0.08	351	298	NA	6	0.9348
0.09	351	298	NA	6	0.9046
0.10	351	298	NA	6	0.9113

Table 7.15: Example 3. Using Hager and Zhang-NR

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	380	311	NA	5	0.9410
0.02	325	282	NA	6	0.8062
0.03	353	283	NA	5	0.8806
0.04	402	337	NA	6	0.9975
0.05	361	300	NA	6	0.9101
0.06	404	331	NA	6	1.0350
0.07	411	341	NA	6	1.0531
0.08	370	320	NA	6	0.9740
0.09	380	311	NA	7	0.9960
0.10	370	297	NA	7	0.9615

Table 7.16: Example 3. Using Hager and Zhang-LS

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	F	F	NA	F	F
0.02	361	295	NA	7	0.9852
0.03	391	346	NA	5	1.0641
0.04	591	392	NA	9	1.5917
0.05	324	282	NA	6	0.8934
0.06	411	348	NA	6	1.1268
0.07	335	273	NA	6	0.9551
0.08	351	294	NA	6	1.0124
0.09	342	292	NA	6	0.9878
0.10	390	331	NA	5	1.0826

Table 7.17: Example 3. Using Hager and Zhang-φ

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	342	293	NA	5	0.8882
0.02	366	301	NA	7	0.9787
0.03	399	336	NA	6	1.0468
0.04	361	295	NA	6	0.9211
0.05	280	267	NA	5	0.7284
0.06	366	296	NA	6	0.9368
0.07	397	331	NA	6	1.0432
0.08	367	317	NA	6	0.9604
0.09	386	316	NA	6	0.9845
0.10	370	297	NA	7	0.9615

Table 7.18: Example 3. Using Hager and Zhang-Brgman Function

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	F	F	F	F	F
0.02	F	F	F	F	F
0.03	3793	3686	72	5	0.6623
0.04	4407	4300	84	6	0.7142
0.05	4458	4351	85	6	0.7405
0.06	380	373	7	6	0.1414
0.07	433	425	8	6	0.1513
0.08	3950	3843	75	6	0.7862
0.09	434	426	8	6	0.1701
0.10	4565	4457	87	7	0.8098

Table 7.19: Example 3. Using Hager and Zhang-Quadratic Function

Method	β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
Hager and Zhang-NR	0.03	347	294	NA	5	0.8730
Hager and Zhang-LS	0.02	325	282	NA	6	0.8062
Hager and Zhang-φ	0.05	324	282	NA	6	0.8934
Hager and Zhang-Breg	0.05	280	267	NA	5	0.7284
Hager and Zhang-Quad	0.06	380	373	7	6	0.1414

Table 7.20: New Results of Example 3.

7.4 Numerical Results for Example 4

Method	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
Hager and Zhang-NR	143	81	NA	1	0.4864
Hager and Zhang-LS	404	224	NA	3	1.4113
Hager and Zhang-φ	198	132	NA	2	0.6776
Hager and Zhang-Bregman	359	217	NA	3	1.2298
Hager and Zhang-Quadratic	15028	14751	146	3	2.1026
Han	386426	382367	3785	41	55.9540
Li and Yuan	3571	2773	NA	786	24.2631

Table 7.21: Results of Example Four

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	143	81	NA	1	0.4990
0.02	143	81	NA	1	0.5012
0.03	143	81	NA	1	0.4989
0.04	143	81	NA	1	0.5053
0.05	143	81	NA	1	0.5181
0.06	143	81	NA	1	0.6047
0.07	143	81	NA	1	0.5391
0.08	143	81	NA	1	0.5017
0.09	143	81	NA	1	0.5194
0.10	143	81	NA	1	0.4994

Table 7.22: Example 4. Using Hager and Zhang-NR

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	234	165	NA	2	0.8231
0.02	349	250	NA	3	1.1807
0.03	349	250	NA	3	1.2101
0.04	386	226	NA	3	1.3014
0.05	404	224	NA	3	1.3848
0.06	302	243	NA	3	1.0854
0.07	243	199	NA	3	0.8474
0.08	294	220	NA	3	1.0695
0.09	302	244	NA	3	1.0911
0.10	271	191	NA	3	0.9510

Table 7.23: Example 4. Using Hager and Zhang-LS

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	80	74	NA	1	0.3298
0.02	244	179	NA	2	0.8964
0.03	213	164	NA	2	0.7726
0.04	204	136	NA	2	0.7447
0.05	198	132	NA	2	0.6955
0.06	302	243	NA	2	0.7074
0.07	243	199	NA	2	0.7181
0.08	294	220	NA	2	0.9658
0.09	302	244	NA	2	1.0016
0.10	271	191	NA	2	0.8200

Table 7.24: Example 4. Using Hager and Zhang-φ

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	228	160	NA	2	0.8111
0.02	185	127	NA	2	0.6477
0.03	182	122	NA	2	0.6384
0.04	316	230	NA	3	1.1214
0.05	359	217	NA	3	1.2792
0.06	280	215	NA	3	0.9896
0.07	310	236	NA	3	1.0853
0.08	252	189	NA	3	0.8773
0.09	207	205	NA	3	1.0186
0.10	272	195	NA	3	0.9625

Table 7.25: Example 4. Using Hager and Zhang-Bregman Function

β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
0.01	10506	10306	102	2	1.5502
0.02	11303	11115	110	2	1.6678
0.03	10693	10509	104	2	1.6954
0.04	16145	15864	157	3	2.1762
0.05	15028	14751	146	3	2.9400
0.06	16039	15763	156	3	2.4297
0.07	15633	15359	152	3	2.3839
0.08	16338	16065	159	3	2.3227
0.09	15933	15661	155	3	2.3171
0.10	15831	15560	154	3	2.4638

Table 7.26: Example 4. Using Hager and Zhang-Quadratic

Method	β	Num Func	Num Grads	Num Hess	Num Iters	Time (secs)
Hager and Zhang-NR	-	143	81	NA	1	0.5
Hager and Zhang-LS	0.01	234	165	NA	2	0.8231
Hager and Zhang-φ	0.01	80	74	NA	1	0.3298
Hager and Zhang-Breg	0.03	182	122	NA	2	0.6384
Hager and Zhang-Quad	0.01	10506	10306	102	2	1.5502

Table 7.27: New Results of Example 4

Bibliography

[1] R. Acar, Identification of the coefficient in elliptic equations, *SIAM J. Control Optim.*, 31 (1993), 1221–1244.

[2] P.N. Anh, L.D. Muu, V.H. Nguyen, J.J. Strodiot, Using the Banach contraction principle to implement the proximal point method for multivalued monotone variational inequalities, *J. Optim. Theory Appl.* 124 (2005), no. 2, 285–306.

[3] R. C. Aster, B. Brian and H.T. Clifford, *Parameter Estimation and Inverse Problems*, Elsevier Academic Press 2005.

[4] D.P. Bersekas, *On the Goldstein-Levitin-Polyak Gradient Projection Method*. IEEE Transactions on Automatic Control, Vol. AC-21, No. 2, pp. 174–184, April 1976.

[5] D. P. Bersekas and J.N. Tsitsikis, *Parallel and distributed Computation, Numerical Method*, Prentice-Hall, London 1989.

[6] D. P. Bertsekas, *Nonlinear Programming, Second Edition*. Authena Scientific, 1999.

[7] F. Colombo and D. Guidetti, An inverse problem for the beam equation with memory with nonhomogeneous boundary conditions, *Inverse Problems*, 24 (2008), no. 6, 065015, 28 pp.

[8] L. F. Demkowicz and J. T. Oden, *Applied Functional Analysis*. CRC Press, 1996.

[9] H. Engl, M. Hanke and A. Neubauer, *Regularization of Inverse Problems* Mathematics and Its Applications, Kluwer Academic Publishers, 2000.

[10] R.E. Ewing and T. Lin, A mixed least-squares method for an inverse problem of a nonlinear beam equation, *Inverse Problems*, 15 (1999), no. 1, 19–32,

[11] R.R. Ferdinand, Numerical scheme approximating solution and parameters in a beam equation, *J. Comput. Appl. Math.*, 161 (2003), no. 2, 469–476,

[12] M.S. Gockenbach and A.A. Khan, Identification of Lamé parameters in linear elasticity: a fixed point approach, *J. Indust. Manag. Optim.,* **1** (4) 487-497 (2005).

[13] M.S. Gockenbach and A.A. Khan, A convex objective functional for elliptic inverse problems. In: Mathematical models and methods for real world systems, K.M. Furuti, M.Z. Nashed and A.H. Siddiqi (eds.), Chapman & Hall/CRC, 389–419, 2005.

[14] M.S. Gockenbach and A.A. Khan, An abstract framework for elliptic inverse problems. Part 1: an output least-squares approach, *Math. Mech. Solids*, **12** (2007), 259-276.

[15] M.S. Gockenbach and A.A. Khan, An abstract framework for elliptic inverse problems. Part 2: an augmented Lagrangian approach, *Mathematics and Mechanics of Solids,* 14, 2009, 517-539

[16] M.S. Gockenbach, B. Jadamba and A.A. Khan, Numerical estimation of discontinuous coefficients by the method of equation error, Inter. J. Math. Comp. Sci. **1** (2006) 343-359.

[17] M.S. Gockenbach, B. Jadamba and A.A. Khan, Equation error approach for elliptic inverse problems with an application to the identification of Lamé parameters, Inverse Problems in Science and Engineering, **16** (2008), 349-367.

[18] W. Hager and H. Zhang, Self-adaptive inexact proximal point methods, *Comput. Optim. Appl.*, 39 (2008), no. 2, 161–181.

[19] D. Han, A new hybrid generalized proximal point algorithm for variational inequality problems, *J. Global Optim.*, 26 (2003), no. 2, 125–140.

[20] D. Han, A generalized proximal-point-based prediction-correction method for variational inequality problems, *J. Comput. Appl. Math.*, 221 (2008), no. 1, 183–193.

[21] J. Hwang, Parameter identification problems for an extensible beam equation, *J. Math. Anal. Appl.*, 359 (2009), no. 2, 682–695.

[22] C. Kanzow, Proximal-like methods for convex minimization problems, Optimization and control with applications, 369–392, Appl. Optim., 96, Springer, New York, 2005.

[23] A. Kaplan and R. Tichatschke, A general view on proximal point methods to variational inequalities in Hilbert spaces–iterative regularization and approximation, *J. Nonlinear Convex Anal.* 2 (2001), no. 3, 305–332,

[24] A. Kaplan and R. Tichatschke, Proximal point method and elliptic regularization, *Nonlinear Anal.* 71 (2009), no. 10, 4525–4543.

[25] C. T. Kelly, *Iterative Methods for Optimization*. SIAM Frontiers in Applied Mathematics, 1999.

[26] D. Kinderleher and G. Stampacchia, *An Introduction to Variational Inequalities and Their Applications*. SIAM Classics In Applied Mathematics, 31, 2000.

[27] K. Kunisch and E. Graif, Parameter estimation for the Euler-Bernoulli beam, *Mat. Apl. Comput.*, 4 (1985), no. 2, 95–124.

[28] K. Kunisch and L.W. White, Regularity properties in parameter estimation of diffusion coefficients in one-dimensional elliptic boundary value problems, *Applicable Anal.*, 21 (1986), no. 1–2.

[29] K. Kunisch and L.W. White, Parameter identifiability under approximation, *Quart. Appl. Math.*, 44 (1986), no. 3, 475–486.

[30] K. Kunisch and L.W. White, Parameter estimation, regularity and the penalty method for a class of two-point boundary value problems, *SIAM J. Control Optim.*, 25 (1987), no. 1, 100–120.

[31] J.J. More, B.S. Garbow and K. E. Hillström, *Testing Unconstrained Optimization Software*, ACM Transactions on Mathematical Software, 7:1, pp 17–41, 1981.

[32] L.A. Parente, P.A. Lotito and M.V. Solodov, A class of inexact variable metric proximal point algorithms, *SIAM J. Optim.*, 19 (2008), no. 1, 240–260.

[33] R.T. Rockafellar, Augmented Lagrangians and applications of the proximal point algorithm in convex programming, *Math. Oper. Res.*, 1 (1976), no. 2, 97–116.

[34] R.T. Rockafellar, Monotone operators and the proximal point algorithm, *SIAM J. Control Optimization*, 14 (1976), no. 5, 877–898.

[35] R. Smith and K. Bowers, A fully Galerkin method for the recovery of stiffness and damping parameters in Euler-Bernoulli beam models, Computation and control, II (Bozeman, MT, 1990), 289–306, Progr. Systems Control Theory, 11, Birkhäuser Boston, Boston, MA, 1991.

[36] P. Tossings, The perturbed proximal point algorithm and some of its applications, *Appl. Math. Optim.*, 29 (1994), no. 2, 125–159.

[37] C.C. Travis and L.W. White, Parameter identification of distributed parameter systems, Math. Biosci. 77 (1985), no. 1–2, 341–352.

[38] L.W. White, Control of beams and plates: location of actuators. Nonlinear analysis and applications (Arlington, Tex., 1986), 599–605, Lecture Notes in Pure and Appl. Math., 109, Dekker, New York, 1987.

[39] L.W. White, Estimation of flexural rigidity in a Kirchhoff plate model, *Appl. Math. Comput.*, 27 (1988), no. 4, part II, 337–359.

[40] L.W. White, Control of beams and plates with small damping: location of actuators, *Appl. Anal.*, 28 (1988), no. 4, 297–327.

[41] L.W. White, Estimation of elastic coefficients in beams with parameter constraints: penalization, *J. Math. Anal. Appl.*, 135 (1988), no. 2, 671–690.

[42] L.W. White, Estimation of elastic parameters in beams and certain plates: H1 regularization, *J. Optim. Theory Appl.* 60 (1989), no. 2, 305–326.

[43] L. W. White, Estimation of higher-order damping terms in linear plate models, *Appl. Math. Comput.* 33 (1989), no. 2, part II, 89–122.

[44] L.W. White, Stability of optimal output least squares estimators in certain beams and plate models, *Appl. Anal.* 39 (1990), no. 1, 15–33.

[45] L.W. White, Estimation of elastic parameters in a nonlinear elliptic model of a plate, *Appl. Math. Comput.*, 42 (1991), no. 2, part II, 139–187.

[46] L.W. White, Estimation of elastic parameters in a von Kármán model, *Nonlinear Anal.*, 18 (1992), no. 9, 829–849.

[47] L.W. White and Y.S. Feng, Estimation of elastic coefficients for a multiple beam structure, *J. Optim. Theory Appl.* 79 (1993), no. 3, 611–640.

[48] L.W White and J. Zhou, Continuity and uniqueness of regularized output least squares optimal estimators, *J. Math. Anal. Appl.* 196 (1995), no. 1, 53–83.

[49] C.R. Vogel, *Computational Methods for Inverse Problems*. Frontiers in Applied Mathematics, SIAM, 2002.

[50] H. Xu, A regularization method for the proximal point algorithm, *J. Global Optim.*, 36 (2006), no. 1, 115–125.