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Numerical Methods for Solving the Inverse Problem of Parameter Identification in Parabolic and Fourth-Order Partial Differential Equations

by
Nathaniel Bush

A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Science in Applied and Computational Mathematics

School of Mathematical Sciences
College of Science

Rochester Institute of Technology
Rochester, NY
Aug 30, 2013

Advisor: Dr. Akhtar A. Khan
Committee: Prof. Dr. Patricia Clark
Dr. Bonnie Jacob
Dr. Baasansuren Jadamba

Abstract

There is a broad range of mathematical problems that can be classified under the title of inverse problems. In this thesis we concern ourselves with the inverse problem of identifying variable coefficients from observation data given an underlying fourth-order or parabolic partial differential equation. We focus on the methods that are employed to derive the gradient of the output least-squares, modified output least-squares, and equation error approach cost functionals. We show the complete derivation of equations, computation of finite element matrices necessary to find the solution of the inverse problem, and display numerical results achieved by numerical implementation of finite element method discretization.

Dedication

I would like to express the deepest appreciation for my thesis advisor, Dr. Akhtar Khan, for his expert guidance. Moreover, I have immense gratitude for his continual dispensing of motivation, selfless actions in all matters, and ability to understand my shortcomings. Without his guidance my thesis would not have been a success.

I would also like to thank my thesis committee members, Dr. Baasansuren Jadamba, Dr. Bonnie Jacob, and Prof. Patricia Clark for their assistance. Furthermore, I thank the amazing group of people that I have worked with under Dr. Akhtar Khan's leadership, especially Brian Winkler, Erin Crossen, Selin Sariaydin, Ben Parker, and Aydar Uatay. Their support was essential to the completion of this thesis.

Committee Approval:

Dr. Akhtar Khan	Date
Thesis Advisor	

Dr. Baasansuren Jadamba	Date
Committee Member	

Dr. Bonnie Jacob	Date
Committee Member	

Prof. Patricia Clark	Date
Committee Member	

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Introduction

There is a broad range of mathematical problems that can be classified under the title of inverse problems. Their main overarching commonality is they involve converting a set of observations of a system into information about the system's unobservable properties. In this thesis we will be concerned with systems that are described by a differential equation and the information we wish to discover are coefficients in the differential equation. We formulate the inverse problem by posing a constrained optimization problem which minimizes a norm of the observation data by choosing the optimal coefficient.

This thesis implements multiple inverse problem formulations involving various cost functionals and methods of calculating the gradient of the cost functionals. We implement the output least-squares, modified output least-squares and equation error cost functionals. We explore inverse problems that involve two separate differential equations: a fourth-order differential equation and parabolic partial differential equation.

In the first chapter we formally define the inverse problem and the direct problem in general terms, define important concepts such as well-posedness, cost functionals, regularization parameters, and discuss the algorithms for solving the inverse problem.

The Second chapter involves solving the inverse problem of identifying a variable coefficient in a fourth-order ordinary differential equation. We show the detailed derivation and solution method for solving the direct problem and the Finite Element Method implementation. We perform a

general derivation of the adjoint stiffness matrix which is used in the computation of the cost functional's gradient. Finally, we show the implementation details and show numerical examples for output least-squares, modified output least-squares and equation error approach.

The third chapter outlines the methods and procedures for deriving and implementing methods for finding a spatially varying coefficient in a general parabolic partial differential equation. We compute the gradient of the output least-squares cost functional by an alternate method to the adjoint stiffness approach and give numerical examples.

This thesis is meant to be self-contained, giving a complete derivation and explanation for all concepts and methods used in solving the inverse problems. The last chapter is an appendix containing definitions of concepts that might not be familiar to undergraduate and graduate students of mathematics.

Chapter 1

Inverse Problem of Coefficient Identification

1.1 Direct Problem and Inverse Problem

Inverse problems arise when our objective is to recover information about a system from observations of the system. The system is usually closed which refers to the property that the information we wish to recover cannot be directly observed.

The direct problem relates a set of model parameters to a solution of the system. The forward operator, the operator defining the direct problem, contains information about the relationship between the model parameters determining what occurs inside the closed system and the measurement of what we observe occurring outside the system. We define the forward operator as $\mathcal{F} : \mathcal{A} \rightarrow D$ where \mathcal{A} is the set of model all possible parameters and D is the set of possible solutions or measurements. The forward problem is defined as:

Find the solution $d \in D$ such that

$$\mathcal{F}(a) = d \tag{1.1}$$

given a specific $a \in \mathcal{A}$.

Conversely, the inverse problem relates the observations outside the system, to model parameters. In inverse problems we are provided with measurement data of our solution, and we are concerned with identifying the correct model parameters. Thus, we can define the inverse problem as:

Find the model parameter $a \in \mathcal{A}$ such that

$$\mathcal{F}(a) = d \tag{1.2}$$

given a specific $d \in D$.

In this paper we will consider models \mathcal{F} to be differential equations, parameters a are coefficients in the differential equations, and d is a possible solution to \mathcal{F} in the context of the forward problem (1.1) and a discrete set of measurement data in the context of the inverse problem (1.2).

The forward operator \mathcal{F} is a differential equation which can be discretized to a finite dimensional system of equations. Therefore the forward problem and inverse problem can be posed as satisfying $\mathcal{F}a = d$ where \mathcal{F} is an $m \times n$ matrix, a is an $n \times 1$ vector, and d is a $m \times 1$ vector.

1.2 Well-posedness

Inverse problems are often difficult to solve because of the issue of ill-posedness [1]. Inverse problems are often ill-posed because there is often more than one choice of coefficient a which allows $\mathcal{F}(a) = d$ to be satisfied. A problem is said to be ill-posed if it fails to be well-posed according the definition provided by Jacques Hadamard in 1902.

A problem is well-posed in the sense of Hadamard if it has the properties that

- i A solution exists.

- ii The solution is unique.
- iii The solution depends continuously on the data.

The last property, perhaps being the most important in finding the solution of an inverse problem, may determine the stability of our solution. If the solution of the problem does not depend continuously on the data then small changes in the data will result in large changes in our solution. Therefore it will be difficult to implement a numerical algorithm to approximate our solution. In this case the problem must be reposed to satisfy the stability requirement. Note that this can be achieved in several ways, one possible method is with the addition of a regularization term which we will utilize in this paper.

1.3 General Inverse Problem Formulation

We present the inverse problem of identifying $a(x)$ as a finite dimensional optimization problem. The solution to the problem is formulated as the minimizer of a cost functional which is defined by the coefficient to solution mapping. The minimization problem has the following form:

$$\min_{a(x) \in \mathcal{A}} J(a) \quad (1.3)$$

where J is a function from \mathcal{A} to \mathbb{R} called the cost functional and \mathcal{A} is the set of admissible coefficients. We want our solution to satisfy the inverse problem condition from the previous section that $\mathcal{F}(a) = d$ where \mathcal{F} is a differential equation model, a is the parameter we wish to identify, and d is the given data. Therefore we can define the cost functional in the above minimization problem as

$$J(a) = ||\mathcal{F}(a) - z||^2 \quad (1.4)$$

for some suitable norm, and z is the discrete set of measurement data.

Since the direct problem is a differential equation, we can reformulate it in its corresponding variational form given by (1.5). Therefore the forward operator is replaced with the solution $u \in \mathcal{V}$ to the variational problem

$$b(u, v) = f(v) \quad \forall v \in \mathcal{V} \quad (1.5)$$

where $b(\cdot, \cdot)$ is the bilinear form and \mathcal{V} is the typical space of test functions defined in variational problems. The optimization approach for the inverse problem has the form

$$\min_{a(x) \in \mathcal{A}} \|u(a) - z\|^2 \quad (1.6)$$

where u is the solution to the variational problem depending on the parameter $a(x)$.

1.4 Regularization

The inverse problem of identifying a spatially varying coefficient in a differential equation is subject to problems of ill-posedness and overfitting. We introduce the process regularization which introduced additional information in order to create a well-posed problem and prevent overfitting. The issue of well-posedness was covered in previous sections. Overfitting occurs when the values of the recovered coefficient are influenced by noise instead of by the underlying model or data. Regularization introduces a tradeoff between fitting the data with the correct coefficient and reducing a norm of the coefficient.

$$\min_{a(x) \in \mathcal{A}} J(a) + \epsilon R(a) \quad (1.7)$$

We redefine the minimization problem by introducing the regularization functional, $R(a)$, and the regularization parameter, ϵ . The regularization parameter is a small positive constant and can be defined in alternate functional forms.

The coefficient we wish to identify is an element of a specific function space of admissible coefficients defined by

$$\mathcal{A} = \{a = a(x) | a \in H^1(\Omega), 0 < k_0 \leq a \leq k_1 < \infty \text{ on } \Omega, k_i \in \mathbb{R}^+\} \quad (1.8)$$

where $a = a(x, y)$ in the case of two dimensions. The regularization functional, $R(a)$, can be defined by one of the following norms.

$$L^2\text{-norm: } \|a\|_{H^0(\Omega)} = \|a\|_{L^2(\Omega)} = \int_{\Omega} |a|^2 \quad (1.9)$$

$$H^1\text{-norm: } \|a\|_{H^1(\Omega)} = \int_{\Omega} |a|^2 + \int_{\Omega} |\nabla a|^2 \quad (1.10)$$

$$H^1\text{-seminorm: } \|a\|_{\tilde{H}^1(\Omega)} = \int_{\Omega} |\nabla a|^2 \quad (1.11)$$

where $\tilde{H}^1(\Omega)$ denotes the semi-norm of $H^1(\Omega)$.

1.5 Inverse Problem Algorithm

In this section we will briefly discuss the inverse problem algorithm that will be implemented in the following chapters. We provide general descriptions of how to solve an inverse problem of identifying a coefficient from observation data. The steps are as follows:

1. Initial guess for the coefficient: $(a_i = a_0)$.
2. Solve the direct problem: Find $u(a_i)$.
3. Evaluate cost functional value: $J(a_i)$.
4. Compute gradient of cost functional: $\nabla J(a_i)$.
5. Using gradient descent algorithm, move in direction of steepest descent: Compute a_{i+1} .
6. Repeat steps 2-6 until stopping criteria is satisfied: $\|\nabla J(a_i)\| < \text{tol}$.

First, an initial guess for the coefficient is provided based on some assumptions of the data. A reasonably good initial guess is required for convergence of the algorithm.

Second, we find the solution of the direct problem from the appropriate differential equation using the provided coefficient.

Next, we use $u(a_i)$ from step 2 to compute the value of the cost functional and the gradient of the cost functional given a_i .

A constrained optimization method, such as a gradient descent algorithm is used to find a_{i+1} which reduces the value of the cost functional. In our numerical examples we will use a conjugate gradient trust region method which uses $J(a_i)$ and $\nabla J(a_i)$ to find a_{i+1} .

We repeat steps 2-6 until the necessary stopping criteria is met. In this case our stopping criteria is the condition that the gradient of the cost functional $\|\nabla J a_i\|$ is less than a pre-defined tolerance level. For example, the pre-defined tolerance level used in our numerical examples is 10^{-12} .

Chapter 2

The Fourth-Order Inverse Problem

In this section we study a general fourth-order differential equation with three spatially varying coefficients. The case of identifying a coefficient in a fourth-order differential equation has an important application in materials science; specifically in modeling the deflection of a beam. This has been studied extensively in several contexts involving beam problems and the related 2-dimensional modeling of car windshields studied in [2] and [3].

2.1 Direct Problem Formulation

In this section we introduce the problem of solving a fourth-order differential equation by finite element methods. The general partial differential equation is

$$\frac{d^2}{dx^2} \left(a(x) \frac{d^2 u}{dx^2} \right) - \frac{d}{dx} \left(b(x) \frac{du}{dx} \right) + c(x)u = f(x), \quad x \in \Omega \quad (2.1)$$

$$u(x) = \frac{du}{dx}(x) = 0 \quad \forall x \in \Gamma \quad (2.2)$$

where f is a real-valued piecewise continuous and bounded function, $\Omega = [0, 1]$ and $\Gamma = \{0, 1\}$. In this problem we have homogeneous Dirichlet and Neumann boundary conditions. These are often called 'clamped' boundary conditions. We define the linear space of test functions as follows:

$$\mathcal{V} = \{v \mid v \text{ and } \frac{dv}{dx} \text{ are continuous on } \Omega, \text{ and } v(x) = \frac{dv}{dx}(x) = 0 \text{ on } \Gamma \} \quad (2.3)$$

We introduce the following inner product notation to be used throughout the thesis which applies to real-valued piecewise continuous and bounded functions.

$$(v, w) = \int_{\Omega} v(x)w(x)dx$$

Next we obtain the weak form, or variational form, of the fourth-order differential equation by distributing test function v through equation (2.1), integrating over Ω , and applying integration by parts with boundary conditions defined by (2.2) and (2.3).

$$\begin{aligned} \int_{\Omega} \frac{d^2}{dx^2} \left(a(x) \frac{d^2 u}{dx^2} \right) v dx - \int_{\Omega} \frac{d}{dx} \left(b(x) \frac{du}{dx} \right) v dx + \int_{\Omega} c(x) u v dx &= \int_{\Omega} f(x) v dx \\ \implies \frac{d}{dx} \left(a(x) \frac{d^2 u}{dx^2} \right) v \Big|_{\Gamma} - \int_{\Omega} \frac{d}{dx} \left(a(x) \frac{d^2 u}{dx^2} \right) \frac{dv}{dx} dx & \\ - b(x) \frac{du}{dx} v \Big|_{\Gamma} + \int_{\Omega} b(x) \frac{du}{dx} \frac{dv}{dx} dx + \int_{\Omega} c(x) u v dx &= \int_{\Omega} f(x) v dx \\ \implies \frac{d}{dx} \left(a(x) \frac{d^2 u}{dx^2} \right) v \Big|_{\Gamma} - a(x) \frac{d^2 u}{dx^2} \frac{dv}{dx} \Big|_{\Gamma} + \int_{\Omega} a(x) \frac{d^2 u}{dx^2} \frac{d^2 v}{dx^2} dx & \\ - b(x) \frac{du}{dx} v \Big|_{\Gamma} + \int_{\Omega} b(x) \frac{du}{dx} \frac{dv}{dx} dx + \int_{\Omega} c(x) u v dx &= \int_{\Omega} f(x) v dx \end{aligned}$$

Using boundary conditions supplied by (2.3) the first two terms of the above equation evaluate to 0. Therefore we have the following equation which we can also write in variational form. Note that this is true for every test function since v was chosen arbitrarily from the linear space.

$$\begin{aligned} \int_{\Omega} a(x) \frac{d^2 u}{dx^2} \frac{d^2 v}{dx^2} dx + \int_{\Omega} b(x) \frac{du}{dx} \frac{dv}{dx} dx + \int_{\Omega} c(x) u v dx &= \int_{\Omega} f(x) v dx \quad \forall v \in \mathcal{V} \\ \implies \left(a(x) \frac{d^2 u}{dx^2}, \frac{d^2 v}{dx^2} \right) + \left(b(x) \frac{du}{dx}, \frac{dv}{dx} \right) + (c(x)u, v) &= (f(x), v) \quad \forall v \in \mathcal{V} \end{aligned}$$

We define \mathcal{V}_h to be a finite dimensional subspace of \mathcal{V} , which is an infinite dimensional space of functions, in order to properly define the finite element discretization of our solution. In the following section we will formally define the corresponding basis functions, matrices, and finite element representation.

2.2 FEM Implementation

2.2.1 Stiffness Matrix Computation

The solution, u , has a unique representation given a basis function representation. The basis function representation is

$$u = \sum_{j=1}^n [u_j \phi_j + \hat{u}_j \psi_j]. \quad (2.4)$$

where u_j represents the coefficients on ϕ_j and \hat{u}_j represents the coefficients on ψ_j .

Substituting the basis function representation of our solution into the weak form equation allows us to put the equation in a form where we can calculate the adjoint stiffness matrix. First we replace the test function v , with each of the basis functions and obtain the following two equations.

$$\begin{aligned} \left(a(x) \sum_{j=1}^n [u_j \phi_j'' + \hat{u}_j \psi_j''], \phi_i'' \right) + \left(b(x) \sum_{j=1}^n [u_j \phi_j' + \hat{u}_j \psi_j'], \phi_i' \right) \\ + \left(c(x) \sum_{j=1}^n [u_j \phi_j' + \hat{u}_j \psi_j], \phi_i \right) = (f_i, \phi_i) \end{aligned} \quad (2.5)$$

$$\begin{aligned} \left(a(x) \sum_{j=1}^n [u_j \phi_j'' + \hat{u}_j \psi_j''], \psi_i'' \right) + \left(b(x) \sum_{j=1}^n [u_j \phi_j' + \hat{u}_j \psi_j'], \psi_i' \right) \\ + \left(c(x) \sum_{j=1}^n [u_j \phi_j' + \hat{u}_j \psi_j], \psi_i \right) = (f_i, \psi_i) \end{aligned} \quad (2.6)$$

where ϕ'' is the derivative $\frac{d^2 \phi}{dx^2}$ and likewise with ψ . We introduce the notation that $\Phi = [\phi, \psi]'$, where $'$ is the transpose operation, so the above two equations condense to the following equation.

$$\begin{aligned} \sum_{j=1}^n u_j A_k (a_k \phi_j'', \Phi_i'') + \sum_{j=1}^n u_j' A_k (a_k \psi_j'', \Phi_i'') + \sum_{j=1}^n u_j B_k (b_k \phi_j', \Phi_i') + \sum_{j=1}^n u_j' B_k (b_k \psi_j', \Phi_i') \\ + \sum_{j=1}^n u_j C_k (c_k \phi_j, \Phi_i) + \sum_{j=1}^n u_j' C_k (c_k \psi_j, \Phi_i) = (f_i, \Phi_i) \end{aligned} \quad (2.7)$$

where we have made a substitution for the coefficients in terms of their basis functions by the equations

$$\begin{aligned}
 a(x) &= \sum_{k=1}^n A_k a_k, \\
 b(x) &= \sum_{k=1}^n B_k b_k, \text{ and} \\
 c(x) &= \sum_{k=1}^n C_k c_k.
 \end{aligned}$$

A_k , B_k , and C_k represent the k^{th} coefficient and a_k , b_k , and c_k represent the k^{th} basis function for the corresponding coefficient. Imposing basis function conditions we can solve for the precise cubic polynomials representing the solution.

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

where I_j is the interval to the left of x_j defined as $I_j = [x_{j-1}, x_j]$ and similarly $I_{j+1} = [x_j, x_{j+1}]$.

The following values are calculated by taking the appropriate derivative and finding the basis function value at the specified point. We also impose the condition that we have a regular mesh (i.e. we have equally spaces nodes over the mesh). These values are necessary for the computation of the stiffness matrix.

$$\begin{aligned}
 \phi_j(x_{j+1}) &= 0 & \phi'_j(x_{j+1}) &= 0 \\
 \phi_j(x_{j-1}) &= 0 & \phi'_j(x_{j-1}) &= 0 \\
 \phi_j(x_{j+1/2}) &= 1/2 & \phi'_j(x_{j+1/2}) &= -\frac{3}{2h} \\
 \phi_j(x_{j-1/2}) &= 1/2 & \phi'_j(x_{j-1/2}) &= \frac{3}{2h} \\
 \phi_j(x_j) &= 1 & \phi'_j(x_j) &= 0
 \end{aligned}$$

$$\phi_j''(x_{j+1}) = \frac{6}{h^2}$$

$$\phi_j''(x_{j-1/2}) = 0$$

$$\phi_j''(x_{j-1}) = \frac{6}{h^2}$$

$$\phi_j''(x_{j+1/2}) = 0$$

$$\phi_j''(x_j) = -\frac{6}{h^2}$$

$$\psi_j(x_{j+1}) = 0$$

$$\psi_j'(x_{j-1/2}) = -\frac{1}{4}$$

$$\psi_j(x_{j-1}) = 0$$

$$\psi_j'(x_j) = 1$$

$$\psi_j(x_{j+1/2}) = h/8$$

$$\psi_j''(x_{j+1}) = \frac{2}{h}$$

$$\psi_j(x_{j-1/2}) = -h/8$$

$$\psi_j''(x_{j-1}) = -\frac{2}{h}$$

$$\psi_j(x_j) = 0$$

$$\psi_j''(x_{j+1/2}) = -\frac{1}{h}$$

$$\psi_j'(x_{j+1}) = 0$$

$$\psi_j''(x_{j-1/2}) = \frac{1}{h}$$

$$\psi_j'(x_{j-1}) = 0$$

$$\lim_{x \rightarrow x_j^-} \psi_j''(x_j) = \frac{4}{h}$$

$$\psi_j'(x_{j+1/2}) = -\frac{1}{4}$$

$$\lim_{x \rightarrow x_j^+} \psi_j''(x_j) = -\frac{4}{h}$$

In the following equations we will derive the values for each entry in the submatrices A , B , C , and D . They will be used to construct the stiffness matrix K as a block matrix.

$$A_{i,j} = (a(x)\phi_j'', \phi_i'')$$

$$G_{i,j} = (a(x)\phi_j'', \psi_i'')$$

$$B_{i,j} = (a(x)\psi_j'', \phi_i'')$$

$$H_{i,j} = (a(x)\psi_j'', \psi_i'')$$

$$C_{i,j} = (b(x)\phi_j', \phi_i')$$

$$I_{i,j} = (b(x)\phi_j', \psi_i')$$

$$D_{i,j} = (b(x)\psi_j', \phi_i')$$

$$J_{i,j} = (b(x)\psi_j', \psi_i')$$

$$E_{i,j} = (c(x)\phi_j, \phi_i)$$

$$K_{i,j} = (c(x)\phi_j, \psi_i)$$

$$F_{i,j} = (c(x)\psi_j, \phi_i)$$

$$L_{i,j} = (c(x)\psi_j, \psi_i)$$

$$K = \begin{pmatrix} A + C + E & B + D + F \\ G + I + K & H + J + L \end{pmatrix} \quad U = \begin{pmatrix} u \\ \hat{u} \end{pmatrix} \quad F = \begin{pmatrix} F_\phi \\ F_\psi \end{pmatrix} \quad (2.8)$$

$$\Rightarrow K(A)U = F \quad (2.9)$$

Note that matrices A , C , E , H , J , and L are symmetric. Also $G = B^T$, $I = D^T$, and $K = F^T$.

Next submatrix of the stiffness matrix, \mathbf{K} , is calculated.

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

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

$$A_{j,j-1} = A_{j-1,j}$$

$$\begin{aligned} B_{j,j} &= (a(x)\psi_j'', \phi_j'') \\ &= \int_{x_{j-1}}^{x_{j+1}} a(x)\psi_j''\phi_j'' dx \end{aligned}$$

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

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

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

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

$$\begin{aligned}
 &= \frac{h}{6} \left(a_{j-1} \left(\frac{4}{h^2} \right) + 4a_{j-\frac{1}{2}} \left(\frac{1}{h^2} \right) + a_j \left(\frac{16}{h^2} \right) \right) + \frac{h}{6} \left(a_j \left(\frac{16}{h^2} \right) + 4a_{j+\frac{1}{2}} \left(\frac{1}{h^2} \right) + a_{j+1} \left(\frac{4}{h^2} \right) \right) \\
 &\approx \frac{2}{3h} \left(k_{j-1} + k_{j-\frac{1}{2}} + 8k_j + k_{j+\frac{1}{2}} + k_{j+1} \right) \\
 &= \frac{1}{h} (k_{j-1} + 6k_j + k_{j+1})
 \end{aligned}$$

$$\begin{aligned}
 H_{j-1,j} &= (a(x)\psi_j'', \psi_{j-1}'') \\
 &= \int_{x_{j-1}}^{x_j} a(x)\psi_{j-1}''\psi_j'' dx \\
 &\approx \frac{h}{6} \left(a_{j-1}\psi_{j-1}''(x_{j-1})\psi_j''(x_{j-1}) + 4a_{j-\frac{1}{2}}\psi_{j-1}''(x_{j-\frac{1}{2}})\psi_j''(x_{j-\frac{1}{2}}) + a_j\psi_{j-1}''(x_j)\psi_j''(x_j) \right) \\
 &= \frac{h}{6} \left(a_{j-1} \left(\frac{8}{h^2} \right) + 4a_{j-\frac{1}{2}} \left(\frac{-1}{h^2} \right) + a_j \left(\frac{8}{h^2} \right) \right) \\
 &= \frac{1}{h} \left(a_{j-1} \frac{8}{h^2} + (a_{j-1} + a_j) \frac{-2}{h^2} + a_j \frac{8}{h^2} \right) \\
 &= \frac{1}{h} (a_{j-1} + a_j)
 \end{aligned}$$

$$H_{j,j-1} = H_{j-1,j}$$

$$\begin{aligned}
 C_{j,j} &= (b(x)\phi_j', \phi_j') \\
 &= \int_{x_{j-1}}^{x_{j+1}} b(x)(\phi_j')^2 dx \\
 &= \int_{x_{j-1}}^{x_j} b(x)(\phi_j')^2 dx + \int_{x_j}^{x_{j+1}} b(x)(\phi_j')^2 dx \\
 &\approx \frac{h}{6} \left(b_{j-1}\phi_j'(x_{j-1})^2 + 4b_{j-\frac{1}{2}}\phi_j'(x_{j-\frac{1}{2}})^2 + b_j\phi_j'(x_j)^2 \right) \\
 &\quad + \frac{h}{6} \left(b_j\phi_j'(x_j)^2 + 4b_{j+\frac{1}{2}}\phi_j'(x_{j+\frac{1}{2}})^2 + b_{j+1}\phi_j'(x_{j+1})^2 \right) \\
 &= \frac{h}{6} \left(0 + 4b_{j-\frac{1}{2}} \left(\frac{9}{4h^2} \right) + 0 \right) + \frac{h}{6} \left(0 + 4b_{j+\frac{1}{2}} \left(\frac{9}{4h^2} \right) + 0 \right) \\
 &= \frac{3}{2h} (b_{j-\frac{1}{2}} + b_{j+\frac{1}{2}}) \\
 &\approx \frac{3}{4h} (b_{j-1} + 2b_j + b_{j+1})
 \end{aligned}$$

$$\begin{aligned}
 C_{j-1,j} &= (b(x)\phi_j', \phi_{j-1}') \\
 &= \int_{x_{j-1}}^{x_{j+1}} b(x)\phi_{j-1}'\phi_j' dx
 \end{aligned}$$

$$\begin{aligned}
 &= \int_{x_{j-1}}^{x_j} b(x) \phi'_{j-1} \phi'_j \, dx + \int_{x_j}^{x_{j+1}} b(x) \phi'_{j-1} \phi'_j \, dx \\
 &\approx \frac{h}{6} \left(b_{j-1} \phi'_{j-1}(x_{j-1}) \phi'_j(x_{j-1}) + 4b_{j-\frac{1}{2}} \phi'_{j-1}(x_{j-\frac{1}{2}}) \phi'_j(x_{j-\frac{1}{2}}) + b_j \phi'_{j-1}(x_j) \phi'_j(x_j) \right) \\
 &= \frac{h}{6} \left(0 + 4b_{j-\frac{1}{2}} \left(\frac{-9}{4h^2} \right) + 0 \right) \\
 &= \frac{-3}{2h} \left(b_{j-\frac{1}{2}} \right) \\
 &\approx \frac{-3}{4h} (b_{j-1} + b_j)
 \end{aligned}$$

$$C_{j,j-1} = C_{j-1,j}$$

$$\begin{aligned}
 D_{j,j} &= (b(x) \psi'_j, \phi'_j) \\
 &= \int_{x_{j-1}}^{x_{j+1}} b(x) \psi'_j \phi'_j \, dx \\
 &= \int_{x_{j-1}}^{x_j} b(x) \psi'_j \phi'_j \, dx + \int_{x_j}^{x_{j+1}} b(x) \psi'_j \phi'_j \, dx \\
 &\approx \frac{h}{6} \left(b_{j-1} \psi'_j(x_{j-1}) \phi'_j(x_{j-1}) + 4b_{j-\frac{1}{2}} \psi'_j(x_{j-\frac{1}{2}}) \phi'_j(x_{j-\frac{1}{2}}) + b_j \psi'_j(x_j) \phi'_j(x_j) \right) \\
 &\quad + \frac{h}{6} \left(b_j \psi'_j(x_j) \phi'_j(x_j) + 4b_{j+\frac{1}{2}} \psi'_j(x_{j+\frac{1}{2}}) \phi'_j(x_{j+\frac{1}{2}}) + b_{j+1} \psi'_j(x_{j+1}) \phi'_j(x_{j+1}) \right) \\
 &= \frac{h}{6} \left(0 + 4b_{j-\frac{1}{2}} \left(\frac{-1}{4} \right) \left(\frac{3}{2h} \right) + 0 \right) + \frac{h}{6} \left(0 + 4b_{j+\frac{1}{2}} \left(\frac{-1}{4} \right) \left(\frac{-3}{2h} \right) + 0 \right) \\
 &= \frac{1}{4} \left(-b_{j-\frac{1}{2}} + b_{j+\frac{1}{2}} \right) \\
 &\approx \frac{1}{8} (-b_{j-1} + b_{j+1})
 \end{aligned}$$

$$\begin{aligned}
 D_{j-1,j} &= (b(x) \psi'_j, \phi'_{j-1}) \\
 &= \int_{x_{j-1}}^{x_{j+1}} b(x) \psi'_j \phi'_{j-1} \, dx \\
 &= \int_{x_{j-1}}^{x_j} b(x) \psi'_j \phi'_{j-1} \, dx + \int_{x_j}^{x_{j+1}} b(x) \psi'_j \phi'_{j-1} \, dx \\
 &\approx \frac{h}{6} \left(b_{j-1} \psi'_j(x_{j-1}) \phi'_{j-1}(x_{j-1}) + 4b_{j-\frac{1}{2}} \psi'_j(x_{j-\frac{1}{2}}) \phi'_{j-1}(x_{j-\frac{1}{2}}) + b_j \psi'_j(x_j) \phi'_{j-1}(x_j) \right) \\
 &= \frac{h}{6} \left(0 + 4b_{j-\frac{1}{2}} \left(\frac{-1}{4} \right) \left(\frac{-3}{2h} \right) + 0 \right) \\
 &= \frac{1}{4} \left(b_{j-\frac{1}{2}} \right)
 \end{aligned}$$

$$\approx \frac{1}{8} (b_{j-1} + b_j)$$

$$\begin{aligned}
 D_{j,j-1} &= (b(x)\psi'_{j-1}, \phi'_j) \\
 &= \int_{x_{j-1}}^{x_{j+1}} b(x)\psi'_{j-1}\phi'_j \, dx \\
 &= \int_{x_{j-1}}^{x_j} b(x)\psi'_{j-1}\phi'_j \, dx + \int_{x_j}^{x_{j+1}} b(x)\psi'_{j-1}\phi'_j \, dx \\
 &\approx \frac{h}{6} \left(b_{j-1}\psi'_{j-1}(x_{j-1})\phi'_j(x_{j-1}) + 4b_{j-\frac{1}{2}}\psi'_{j-1}(x_{j-\frac{1}{2}})\phi'_j(x_{j-\frac{1}{2}}) + b_j\psi'_{j-1}(x_j)\phi'_j(x_j) \right) \\
 &= \frac{h}{6} \left(0 + 4b_{j-\frac{1}{2}} \left(\frac{-1}{4} \right) \left(\frac{3}{2h} \right) + 0 \right) \\
 &= \frac{-1}{4} \left(b_{j-\frac{1}{2}} \right) \\
 &\approx \frac{-1}{8} (b_{j-1} + b_j)
 \end{aligned}$$

$$\begin{aligned}
 J_{j,j} &= (b(x)\psi'_j, \psi'_j) \\
 &= \int_{x_{j-1}}^{x_{j+1}} b(x)(\psi'_j)^2 \, dx \\
 &= \int_{x_{j-1}}^{x_j} b(x)(\psi'_j)^2 \, dx + \int_{x_j}^{x_{j+1}} b(x)(\psi'_j)^2 \, dx \\
 &\approx \frac{h}{6} \left(b_{j-1}\psi'_j(x_{j-1})^2 + 4b_{j-\frac{1}{2}}\psi'_j(x_{j-\frac{1}{2}})^2 + b_j\psi'_j(x_j)^2 \right) \\
 &\quad + \frac{h}{6} \left(b_j\psi'_j(x_j)^2 + 4b_{j+\frac{1}{2}}\psi'_j(x_{j+\frac{1}{2}})^2 + b_{j+1}\psi'_j(x_{j+1})^2 \right) \\
 &= \frac{h}{6} \left(0 + 4b_{j-\frac{1}{2}} \left(\frac{1}{16} \right) + b_j \right) + \frac{h}{6} \left(b_j + 4b_{j+\frac{1}{2}} \left(\frac{1}{16} \right) + 0 \right) \\
 &= \frac{h}{24} \left(b_{j-\frac{1}{2}} + 8b_j + b_{j+\frac{1}{2}} \right) \\
 &\approx \frac{h}{48} (b_{j-1} + 18b_j + b_{j+1})
 \end{aligned}$$

$$\begin{aligned}
 J_{j-1,j} &= (b(x)\psi'_j, \psi'_{j-1}) \\
 &= \int_{x_{j-1}}^{x_{j+1}} b(x)\psi'_{j-1}\psi'_j \, dx \\
 &= \int_{x_{j-1}}^{x_j} b(x)\psi'_{j-1}\psi'_j \, dx + \int_{x_j}^{x_{j+1}} b(x)\psi'_{j-1}\psi'_j \, dx \\
 &\approx \frac{h}{6} \left(b_{j-1}\psi'_{j-1}(x_{j-1})\psi'_j(x_{j-1}) + 4b_{j-\frac{1}{2}}\psi'_{j-1}(x_{j-\frac{1}{2}})\psi'_j(x_{j-\frac{1}{2}}) + b_j\psi'_{j-1}(x_j)\psi'_j(x_j) \right)
 \end{aligned}$$

$$\begin{aligned}
 &= \frac{h}{6} \left(0 + 4b_{j-\frac{1}{2}} \left(\frac{1}{16} \right) + 0 \right) \\
 &= \frac{h}{24} \left(b_{j-\frac{1}{2}} \right) \\
 &\approx \frac{h}{48} (b_{j-1} + b_j)
 \end{aligned}$$

$$J_{j,j-1} = J_{j-1,j}$$

$$\begin{aligned}
 E_{j,j} &= (c(x)\phi_j, \phi_j) \\
 &= \int_{x_{j-1}}^{x_{j+1}} c(x)(\phi_j)^2 dx \\
 &= \int_{x_{j-1}}^{x_j} c(x)(\phi_j)^2 dx + \int_{x_j}^{x_{j+1}} c(x)(\phi_j)^2 dx \\
 &\approx \frac{h}{6} \left(c_{j-1}\phi_j(x_{j-1})^2 + 4c_{j-\frac{1}{2}}\phi_j(x_{j-\frac{1}{2}})^2 + c_j\phi_j(x_j)^2 \right) \\
 &\quad + \frac{h}{6} \left(c_j\phi_j(x_j)^2 + 4c_{j+\frac{1}{2}}\phi_j(x_{j+\frac{1}{2}})^2 + c_{j+1}\phi_j(x_{j+1})^2 \right) \\
 &= \frac{h}{6} \left(0 + 4c_{j-\frac{1}{2}} \left(\frac{1}{4} \right) + c_j \right) + \frac{h}{6} \left(c_j + 4c_{j+\frac{1}{2}} \left(\frac{1}{4} \right) + 0 \right) \\
 &= \frac{h}{6} \left(c_{j-\frac{1}{2}} + 2c_j + c_{j+\frac{1}{2}} \right) \\
 &\approx \frac{h}{12} (c_{j-1} + 6c_j + c_{j+1})
 \end{aligned}$$

$$\begin{aligned}
 E_{j-1,j} &= (c(x)\phi_j, \phi_{j-1}) \\
 &= \int_{x_{j-1}}^{x_{j+1}} c(x)\phi_{j-1}\phi_j dx \\
 &= \int_{x_{j-1}}^{x_j} c(x)\phi_{j-1}\phi_j dx + \int_{x_j}^{x_{j+1}} c(x)\phi_{j-1}\phi_j dx \\
 &\approx \frac{h}{6} \left(c_{j-1}\phi_{j-1}(x_{j-1})\phi_j(x_{j-1}) + 4c_{j-\frac{1}{2}}\phi_{j-1}(x_{j-\frac{1}{2}})\phi_j(x_{j-\frac{1}{2}}) + c_j\phi_{j-1}(x_j)\phi_j(x_j) \right) \\
 &= \frac{h}{6} \left(0 + 4c_{j-\frac{1}{2}} \left(\frac{1}{4} \right) + 0 \right) \\
 &= \frac{h}{6} \left(c_{j-\frac{1}{2}} \right) \\
 &\approx \frac{h}{12} (c_{j-1} + c_j)
 \end{aligned}$$

$$E_{j,j-1} = E_{j-1,j}$$

$$\begin{aligned}
 F_{j,j} &= (c(x)\psi_j, \phi_j) \\
 &= \int_{x_{j-1}}^{x_{j+1}} c(x)\psi_j\phi_j \, dx \\
 &= \int_{x_{j-1}}^{x_j} c(x)\psi_j\phi_j \, dx + \int_{x_j}^{x_{j+1}} c(x)\psi_j\phi_j \, dx \\
 &\approx \frac{h}{6} \left(c_{j-1}\psi_j(x_{j-1})\phi_j(x_{j-1}) + 4c_{j-\frac{1}{2}}\psi_j(x_{j-\frac{1}{2}})\phi_j(x_{j-\frac{1}{2}}) + c_j\psi_j(x_j)\phi_j(x_j) \right) \\
 &\quad + \frac{h}{6} \left(c_j\psi_j(x_j)\phi_j(x_j) + 4c_{j+\frac{1}{2}}\psi_j(x_{j+\frac{1}{2}})\phi_j(x_{j+\frac{1}{2}}) + c_{j+1}\psi_j(x_{j+1})\phi_j(x_{j+1}) \right) \\
 &= \frac{h}{6} \left(0 + 4c_{j-\frac{1}{2}} \left(\frac{-h}{8} \right) \left(\frac{1}{2} \right) + 0 \right) + \frac{h}{6} \left(0 + 4c_{j+\frac{1}{2}} \left(\frac{h}{8} \right) \left(\frac{1}{2} \right) + 0 \right) \\
 &= \frac{h^2}{24} \left(-c_{j-\frac{1}{2}} + c_{j+\frac{1}{2}} \right) \\
 &\approx \frac{h^2}{48} (-c_{j-1} + c_{j+1})
 \end{aligned}$$

$$\begin{aligned}
 F_{j-1,j} &= (c(x)\psi_j, \phi_{j-1}) \\
 &= \int_{x_{j-1}}^{x_{j+1}} c(x)\psi_j\phi_{j-1} \, dx \\
 &= \int_{x_{j-1}}^{x_j} c(x)\psi_j\phi_{j-1} \, dx + \int_{x_j}^{x_{j+1}} c(x)\psi_j\phi_{j-1} \, dx \\
 &\approx \frac{h}{6} \left(c_{j-1}\psi_j(x_{j-1})\phi_{j-1}(x_{j-1}) + 4c_{j-\frac{1}{2}}\psi_j(x_{j-\frac{1}{2}})\phi_{j-1}(x_{j-\frac{1}{2}}) + c_j\psi_j(x_j)\phi_{j-1}(x_j) \right) \\
 &= \frac{h}{6} \left(0 + 4c_{j-\frac{1}{2}} \left(\frac{-h}{8} \right) \left(\frac{1}{2} \right) + 0 \right) \\
 &= \frac{-h^2}{24} \left(c_{j-\frac{1}{2}} \right) \\
 &\approx \frac{-h^2}{48} (c_{j-1} + c_j)
 \end{aligned}$$

$$\begin{aligned}
 F_{j,j-1} &= (c(x)\psi_{j-1}, \phi_j) \\
 &= \int_{x_{j-1}}^{x_{j+1}} c(x)\psi_{j-1}\phi_j \, dx \\
 &= \int_{x_{j-1}}^{x_j} c(x)\psi_{j-1}\phi_j \, dx + \int_{x_j}^{x_{j+1}} c(x)\psi_{j-1}\phi_j \, dx \\
 &\approx \frac{h}{6} \left(c_{j-1}\psi_{j-1}(x_{j-1})\phi_j(x_{j-1}) + 4c_{j-\frac{1}{2}}\psi_{j-1}(x_{j-\frac{1}{2}})\phi_j(x_{j-\frac{1}{2}}) + c_j\psi_{j-1}(x_j)\phi_j(x_j) \right) \\
 &= \frac{h}{6} \left(0 + 4c_{j-\frac{1}{2}} \left(\frac{h}{8} \right) \left(\frac{1}{2} \right) + 0 \right)
 \end{aligned}$$

$$\begin{aligned}
 &= \frac{h^2}{24} \left(c_{j-\frac{1}{2}} \right) \\
 &\approx \frac{h^2}{48} (c_{j-1} + c_j)
 \end{aligned}$$

$$\begin{aligned}
 L_{j,j} &= (c(x)\psi_j, \psi_j) \\
 &= \int_{x_{j-1}}^{x_{j+1}} c(x)(\psi_j)^2 dx \\
 &= \int_{x_{j-1}}^{x_j} c(x)(\psi_j)^2 dx + \int_{x_j}^{x_{j+1}} c(x)(\psi_j)^2 dx \\
 &\approx \frac{h}{6} \left(c_{j-1}\psi_j(x_{j-1})^2 + 4c_{j-\frac{1}{2}}\psi_j(x_{j-\frac{1}{2}})^2 + c_j\psi_j(x_j)^2 \right) \\
 &\quad + \frac{h}{6} \left(c_j\psi_j(x_j)^2 + 4c_{j+\frac{1}{2}}\psi_j(x_{j+\frac{1}{2}})^2 + c_{j+1}\psi_j(x_{j+1})^2 \right) \\
 &= \frac{h}{6} \left(0 + 4c_{j-\frac{1}{2}} \left(\frac{h^2}{64} \right) + 0 \right) + \frac{h}{6} \left(0 + 4c_{j+\frac{1}{2}} \left(\frac{h^2}{64} \right) + 0 \right) \\
 &= \frac{h^3}{96} (c_{j-\frac{1}{2}} + c_{j+\frac{1}{2}}) \\
 &\approx \frac{h^3}{192} \left(c_{j-1} + 2c_j + \frac{64}{h^2}c_j + c_{j+1} \right)
 \end{aligned}$$

$$\begin{aligned}
 L_{j-1,j} &= (c(x)\psi_j, \psi_{j-1}) \\
 &= \int_{x_{j-1}}^{x_{j+1}} c(x)\psi_{j-1}\psi_j dx \\
 &= \int_{x_{j-1}}^{x_j} c(x)\psi_{j-1}\psi_j dx + \int_{x_j}^{x_{j+1}} c(x)\psi_{j-1}\psi_j dx \\
 &\approx \frac{h}{6} \left(c_{j-1}\psi_{j-1}(x_{j-1})\psi_j(x_{j-1}) + 4c_{j-\frac{1}{2}}\psi_{j-1}(x_{j-\frac{1}{2}})\psi_j(x_{j-\frac{1}{2}}) + c_j\psi_{j-1}(x_j)\psi_j(x_j) \right) \\
 &= \frac{h}{6} \left(0 + 4c_{j-\frac{1}{2}} \left(\frac{-h^2}{64} \right) + 0 \right) \\
 &= \frac{-h^3}{96} (c_{j-\frac{1}{2}}) \\
 &\approx \frac{-h^3}{192} (c_{j-1} + c_j)
 \end{aligned}$$

$$L_{j,j-1} = L_{j-1,j}$$

2.2.2 Load Vector Computation

In this section we compute the fourth order load vector which is constructed by $F = (F_\phi, F_\psi)$ where $F_\phi = (f, \phi_j)_{j=1,2,\dots,n}$ and $F_\psi = (f, \psi_j)_{j=1,2,\dots,n}$. In the following derivations we use the definition of the load vector and numerically approximate the integrals with Simpson's rule.

$$\begin{aligned}
 (F_\phi)_j &= \int_0^1 f \phi_j dx \\
 &= \int_{x_{j-1}}^{x_j} f \phi_j dx + \int_{x_j}^{x_{j+1}} f \phi_j dx \\
 &= \frac{h_j}{6} [f(x_{j-1})\phi_j(x_{j-1}) + 4f(x_{j-1/2})\phi_j(x_{j-1/2}) + f(x_j)\phi_j(x_j)] \\
 &\quad + \frac{h_{j+1}}{6} [f(x_j)\phi_j(x_j) + 4f(x_{j+1/2})\phi_j(x_{j+1/2}) + f(x_{j+1})\phi_j(x_{j+1})] \\
 &= \frac{h_j}{6} [2f(x_{j-1/2}) + f(x_j)] + \frac{h_{j+1}}{6} [f(x_j) + 2f(x_{j+1/2})]
 \end{aligned}$$

If the mesh is sufficiently fine (i.e. n is sufficiently large) then we can approximate $f(x_{j-1/2})$ and $f(x_{j+1/2})$ by $f(x_j)$.

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

$$\begin{aligned}
 (F_\psi)_j &= \int_0^1 f \psi_j dx \\
 &= \int_{x_{j-1}}^{x_j} f \psi_j dx + \int_{x_j}^{x_{j+1}} f \psi_j dx \\
 &= \frac{h_j}{6} [f(x_{j-1})\psi_j(x_{j-1}) + 4f(x_{j-1/2})\psi_j(x_{j-1/2}) + f(x_j)\psi_j(x_j)] \\
 &\quad + \frac{h_{j+1}}{6} [f(x_j)\psi_j(x_j) + 4f(x_{j+1/2})\psi_j(x_{j+1/2}) + f(x_{j+1})\psi_j(x_{j+1})] \\
 &= -\frac{h_j^2}{12} f(x_{j-1/2}) + h_{j+1} h_j f(x_{j+1/2}) \\
 &= \frac{h_j}{12} [-h_j f(x_{j-1/2}) + h_{j+1} f(x_{j+1/2})]
 \end{aligned}$$

2.2.3 Mass Matrix Computation

In this section we derive the fourth-order mass matrix used in computation of cost functionals and the gradient of cost functionals. The calculation requires much algebra so many steps are omitted for to keep the explanation concise. The integrals in this section are computed exactly by integrating and substituting $x_{j-1} = x_j - h$ or $x_{j+1} = x_j + h$.

$$M = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix} \quad (2.10)$$

$$A_{i,j} = \int_0^1 \phi_i \phi_j dx$$

$$\begin{aligned} A_{j,j} &= \int_0^1 \phi_j \phi_j dx \\ &= \int_{x_{j-1}}^{x_j} \phi_j^2 dx + \int_{x_j}^{x_{j+1}} \phi_j^2 dx \\ &= \frac{13}{35} \frac{h^7}{h^6} + \frac{13}{35} \frac{h^7}{h^6} \\ &= \frac{26}{35} h \end{aligned}$$

$$\begin{aligned} A_{j-1,j} &= \int_0^1 \phi_{j-1} \phi_j dx \\ &= \int_{x_{j-1}}^{x_j} \phi_j \phi_{j-1} dx \\ &= \frac{9}{70} h \end{aligned}$$

$$A_{j,j-1} = A_{j-1,j}$$

$$B_{i,j} = \int_0^1 \phi_i \psi_j dx$$

$$\begin{aligned} B_{j,j} &= \int_0^1 \phi_j \psi_j dx \\ &= \int_{x_{j-1}}^{x_j} \phi_j \psi_j dx + \int_{x_j}^{x_{j+1}} \phi_j \psi_j dx \\ &= 0 \end{aligned}$$

$$\begin{aligned}
 B_{j-1,j} &= \int_0^1 \phi_{j-1} \psi_j dx \\
 &= \int_{x_{j-1}}^{x_j} \phi_{j-1} \psi_j dx \\
 &= \frac{-13}{420} h^2
 \end{aligned}$$

$$\begin{aligned}
 B_{j,j-1} &= \int_0^1 \phi_j \psi_{j-1} dx \\
 &= \int_{x_{j-1}}^{x_j} \phi_j \psi_{j-1} dx \\
 &= \frac{13}{420} h^2
 \end{aligned}$$

$$C_{i,j} = \int_0^1 \psi_i \psi_j dx$$

$$\begin{aligned}
 C_{j,j} &= \int_0^1 \psi_j \psi_j dx \\
 &= \int_{x_{j-1}}^{x_j} \psi_j^2 dx + \int_{x_j}^{x_{j+1}} \psi_j^2 dx \\
 &= \frac{1}{105} \frac{h^7}{h^4} + \frac{1}{105} \frac{h^7}{h^4} \\
 &= \frac{2}{105} \frac{h^7}{h^4}
 \end{aligned}$$

$$\begin{aligned}
 C_{j-1,j} &= \int_0^1 \psi_{j-1} \psi_j dx \\
 &= \int_{x_{j-1}}^{x_j} \psi_j \psi_{j-1} dx \\
 &= \frac{-1}{140} h^3
 \end{aligned}$$

$$C_{j,j-1} = C_{j-1,j}$$

2.3 Inverse Problem Formulation

We introduce a modification of the standard fourth order inverse problem. The problem becomes that of identifying three spacial variable coefficients $a(x)$, $b(x)$ and $c(x)$ in a fourth-order differential equation. The equation in one spacial dimension is given by

$$\frac{d^2}{dx^2} \left(a(x) \frac{d^2 u(x)}{dx^2} \right) - \frac{d}{dx} \left(b(x) \frac{du(x)}{dx} \right) + c(x)u(x) = f(x) \quad (2.11)$$

where the problem is defined on the domain $\Omega = [0, 1]$.

The weak form of the differential equation is obtained as in the previous section by integrating by parts twice and applying boundary conditions. We find the variational form to be

$$\left(a(x) \frac{d^2 u}{dx^2}, \frac{d^2 v}{dx^2} \right) + \left(b(x) \frac{du}{dx}, \frac{dv}{dx} \right) + (c(x)u, v) = (f, v) \quad \forall v \in \mathcal{V}. \quad (2.12)$$

After we obtain the solution to the direct problem, which was formulated above, we move on to finding a fourth-order discretization of the necessary matrices and elements to minimize the cost functional.

2.3.1 The Fréchet derivative of the parameter to solution operator for fourth-order equations

The parameter to solution mapping is defined as $F : \mathcal{A} \rightarrow \mathcal{V}$ where the solution belongs to \mathcal{V} , a Hilbert space, and the parameter belongs to \mathcal{A} , a Banach space.

The trilinear form comes from the variational form of the problem defined in (2.12). We adopt the notation that $q = (a(x), b(x), c(x))$. So given that the trilinear form is defined as

$$T(q, u, v) := \left(a(x) \frac{d^2 u}{dx^2}, \frac{d^2 v}{dx^2} \right) + \left(b(x) \frac{du}{dx}, \frac{dv}{dx} \right) + (c(x)u, v) \quad (2.13)$$

then we have

$$T(q, u, v) = (f, v) \quad \forall v \in \mathcal{V}. \quad (2.14)$$

We find the Fréchet Derivative of the parameter to solution mapping. Let $q \in \text{int}(\mathcal{A})$ and δq be a perturbation on q such that $q + \delta q \in \mathcal{A}$. Also define $\delta w = F(q + \delta q) - F(q)$ and $u = F(q)$. Note that we can write $F(q + \delta q)$ as $u + \delta w$.

The variational form at q has the form

$$T(q, u, v) = (f, v) \quad \forall v \in \mathcal{V} \quad (2.15)$$

and the variational form at $q + \delta q$ has the form

$$T(q + \delta q, u + \delta w, v) = (f, v) \quad \forall v \in \mathcal{V} \quad (2.16)$$

Next, we subtract (2.16) from (2.15) and simplify.

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

Note that the last equation is in the form of the Fréchet Derivative (4.10) which suggests the form of the derivative $DF(q)$. We see that the derivative of our solution is $\delta u = DF(q)\delta q$ and is found by solving the variational equation

$$T(q, \delta u, v) = -T(\delta q, u, v) \quad \forall v \in \mathcal{V}. \quad (2.17)$$

Note that the validity of this argument is not proved here. For a rigorous proof and derivation of this we refer to [4]. For the particular problem we are considering this result translates into the following equation.

$$\left(a \frac{d^2 \delta u}{dx^2}, \frac{d^2 v}{dx^2} \right) + \left(b \frac{d \delta u}{dx}, \frac{dv}{dx} \right) + (c \delta u, v) = \left(\delta a \frac{d^2 u}{dx^2}, \frac{d^2 v}{dx^2} \right) + \left(\delta b \frac{du}{dx}, \frac{dv}{dx} \right) + (\delta c u, v) \quad (2.18)$$

2.3.2 Derivative of $U(A)$

The matrix $U(A)$ is the solution to direct problem discretized by finite element method. We find δU in order to complete the calculation of the derivative of $J(A)$ in the following sections. We begin with the direct problem

$$K(A)U = F. \quad (2.19)$$

Next, we take the derivative of the above matrix equation. Utilizing chain rule and product rule we obtain

$$(DK(A)\delta A)U + K(A)\delta U = 0. \quad (2.20)$$

We use the linearity of $K(A)$ to simplify the expression and obtain an expression for δU .

$$\begin{aligned} (DK(A)\delta A)U + K(A)\delta U &= 0 \\ \implies K(A)\delta U &= -DK(A)(\delta A)U \\ \implies K(A)\delta U &= -K(\delta A)U \\ \implies \delta U &= -K(A)^{-1}K(\delta A)U \end{aligned} \quad (2.22)$$

2.3.3 Adjoint Stiffness Derivation

Here we derive the fourth-order adjoint stiffness matrix in general form from the definition of the stiffness matrix. As before we use cubic basis functions for the solution space and piecewise linear basis functions for the coefficient space. By definition of the the finite dimensional subspace of linear test functions we see that $v \in V_h$ has the form

$$v = \sum_{j=1}^n [v_j \Phi_j + v'_j \Psi_j] \quad (2.23)$$

and we impose the condition that the coefficients have the form

$$a(x) = \sum_{k=1}^m A_k a_k, \quad b(x) = \sum_{k=1}^m B_k b_k \quad \text{and} \quad c(x) = \sum_{k=1}^m C_k c_k. \quad (2.24)$$

where we $m = n + 2$. Also, note that a_k , b_k and c_k are the k^{th} basis functions and A_k , B_k and C_k are coefficients on the k^{th} basis functions for $a(x)$, $b(x)$ and $c(x)$ respectively. Moreover, we adopt the notation that $A = [A_k]$, $B = [B_k]$ and $C = [C_k]$ for $k = 1, 2, \dots, m$. We create a coefficient vector from these coefficients given as

$$Q = \begin{pmatrix} A \\ B \\ C \end{pmatrix} \quad (2.25)$$

We simplify the computations by introducing the simplifications that $\bar{\Phi} = (\Phi, \Psi)^T$ where $\Phi = (\phi_1, \phi_2, \dots, \phi_n)$ and $\Psi = (\psi_1, \psi_2, \dots, \psi_n)$.

$$[K(Q)]_{ij} = \int_{\Omega} a(x) \bar{\Phi}_j'' \bar{\Phi}_i'' dx + \int_{\Omega} b(x) \bar{\Phi}_j' \bar{\Phi}_i' dx + \int_{\Omega} c(x) \bar{\Phi}_j \bar{\Phi}_i dx \quad (2.26)$$

$$\begin{aligned} &= \int_{\Omega} \left(\sum_{k=1}^m A_k a_k \right) \bar{\Phi}_j'' \bar{\Phi}_i'' dx + \left(\sum_{k=1}^m B_k b_k \right) \bar{\Phi}_j' \bar{\Phi}_i' dx + \left(\sum_{k=1}^m C_k c_k \right) \bar{\Phi}_j \bar{\Phi}_i dx \\ &= \sum_{k=1}^m \left(\int_{\Omega} a_k \bar{\Phi}_j'' \bar{\Phi}_i'' dx A_k + \int_{\Omega} b_k \bar{\Phi}_j' \bar{\Phi}_i' dx B_k + \int_{\Omega} c_k \bar{\Phi}_j \bar{\Phi}_i dx C_k \right) \\ [K(Q)\tilde{V}]_i &= \sum_{j=1}^n \left(\sum_{k=1}^m \left(\int_{\Omega} a_k \bar{\Phi}_j'' \bar{\Phi}_i'' dx A_k + \int_{\Omega} b_k \bar{\Phi}_j' \bar{\Phi}_i' dx B_k + \int_{\Omega} c_k \bar{\Phi}_j \bar{\Phi}_i dx C_k \right) \right) \tilde{V}_j \\ &= \sum_{k=1}^m \sum_{j=1}^n \left(\int_{\Omega} a_k \bar{\Phi}_j'' \bar{\Phi}_i'' dx A_k \tilde{V}_j + \int_{\Omega} b_k \bar{\Phi}_j' \bar{\Phi}_i' dx B_k \tilde{V}_j + \int_{\Omega} c_k \bar{\Phi}_j \bar{\Phi}_i dx C_k \tilde{V}_j \right) \end{aligned} \quad (2.27)$$

We adopt the notation that $\tilde{V} = \begin{bmatrix} V & V' \end{bmatrix}^T$ and

$$T_{ijk} = \int_{\Omega} a_k \bar{\Phi}_j'' \bar{\Phi}_i'' dx + \int_{\Omega} b_k \bar{\Phi}_j' \bar{\Phi}_i' dx + \int_{\Omega} c_k \bar{\Phi}_j \bar{\Phi}_i dx. \quad (2.28)$$

Furthermore,

$$[K(Q)\tilde{V}]_i = \sum_{j=1}^n \left(\sum_{k=1}^m T_{ijk} Q_k \right) \tilde{V}_j = \sum_{k=1}^m \left(\sum_{j=1}^n T_{ijk} \tilde{V}_j \right) Q_k = [\mathbf{L}(\tilde{V})Q]_i \quad (2.29)$$

The matrix $\mathbf{L} = \mathbf{L}(\tilde{V})$ is known as the adjoint stiffness matrix. We have shown that it must follow the condition that

$$\mathbf{L}(\tilde{V})Q = K(Q)\tilde{V}, \quad \forall A \in \mathbb{R}^m, \quad \forall \tilde{V} \in \mathbb{R}^{2n}. \quad (2.30)$$

Furthermore, we shown the exact form of the adjoint stiffness matrix.

$$\begin{aligned} [\mathbf{L}(\tilde{V})]_{ik} &= \sum_{j=1}^{2n} T_{ijk} \tilde{V}_j \\ &= \sum_{j=1}^{2n} \left(\int_{\Omega} a_k \bar{\Phi}_j'' \bar{\Phi}_i'' dx + \int_{\Omega} b_k \bar{\Phi}_j' \bar{\Phi}_i' dx + \int_{\Omega} c_k \bar{\Phi}_j \bar{\Phi}_i dx \right) \tilde{V}_j \\ &= \sum_{j=1}^n \left(\int_{\Omega} a_k \bar{\Phi}_j'' \bar{\Phi}_i'' dx + \int_{\Omega} b_k \bar{\Phi}_j' \bar{\Phi}_i' dx + \int_{\Omega} c_k \bar{\Phi}_j \bar{\Phi}_i dx \right) V_j \\ &\quad + \sum_{j=1}^{2n} \left(\int_{\Omega} a_k \bar{\Phi}_j'' \bar{\Phi}_i'' dx + \int_{\Omega} b_k \bar{\Phi}_j' \bar{\Phi}_i' dx + \int_{\Omega} c_k \bar{\Phi}_j \bar{\Phi}_i dx \right) V_j' \end{aligned} \quad (2.31)$$

for all $i = 1, 2, \dots, 2n$ and $k = 1, 2, \dots, m$.

2.3.4 Adjoint Stiffness Matrix Computation

In this section we construct the adjoint stiffness matrix \mathbf{L} by first creating submatrices A , B , C , and D (which are different from the A , B , C , and D in the previous section). These are used to create the \mathbf{L} in the following manner.

$$\begin{aligned}
 A_{i,k} &= \sum_{j=1}^n \left(\int_0^1 a_k \phi_j'' \phi_i'' dx \right) V_j & G_{i,k} &= \sum_{j=1}^n \left(\int_0^1 a_k \phi_j'' \psi_i'' dx \right) V_j \\
 B_{i,k} &= \sum_{j=1}^n \left(\int_0^1 a_k \psi_j'' \phi_i'' dx \right) V_j' & H_{i,k} &= \sum_{j=1}^n \left(\int_0^1 a_k \psi_j'' \psi_i'' dx \right) V_j' \\
 C_{i,k} &= \sum_{j=1}^n \left(\int_0^1 b_k \phi_j' \phi_i' dx \right) V_j & I_{i,k} &= \sum_{j=1}^n \left(\int_0^1 b_k \phi_j' \psi_i' dx \right) V_j \\
 D_{i,k} &= \sum_{j=1}^n \left(\int_0^1 b_k \psi_j' \phi_i' dx \right) V_j' & J_{i,k} &= \sum_{j=1}^n \left(\int_0^1 b_k \psi_j' \psi_i' dx \right) V_j' \\
 E_{i,k} &= \sum_{j=1}^n \left(\int_0^1 c_k \phi_j \phi_i dx \right) V_j & K_{i,k} &= \sum_{j=1}^n \left(\int_0^1 c_k \phi_j \psi_i dx \right) V_j \\
 F_{i,k} &= \sum_{j=1}^n \left(\int_0^1 c_k \psi_j \phi_i dx \right) V_j' & L_{i,k} &= \sum_{j=1}^n \left(\int_0^1 c_k \psi_j \psi_i dx \right) V_j'
 \end{aligned}$$

$$\begin{aligned}
 \mathbf{L} &= \begin{pmatrix} A+B & C+D & E+F \\ G+H & I+J & K+L \end{pmatrix} \\
 &\Rightarrow \mathbf{L}(U)Q = K(Q)U
 \end{aligned}$$

We construct the submatrices of \mathbf{L} by deriving each term of the matrices. We proceed by identifying the intervals of compact support on which we integrate, we numerically approximate the individual integrals by applying Simpson's rule.

$$\begin{aligned}
 A_{i,k} &= \sum_{j=1}^n \left(\int_0^1 a_k \phi_j'' \phi_i'' dx \right) V_j \\
 A_{1,0} &= \sum_{j=1}^n \left(\int_0^1 a_0 \phi_j'' \phi_1'' dx \right) V_j
 \end{aligned}$$

$$\begin{aligned}
 &= \left(\int_0^1 a_0(\phi_1'')^2 dx \right) V_1 \\
 &= \left(\int_{I_1} a_0(\phi_1'')^2 dx \right) V_1 \\
 &= \frac{6}{h^3} V_1 \\
 A_{1,1} &= \sum_{j=1}^n \left(\int_0^1 a_1 \phi_j'' \phi_1'' dx \right) V_j \\
 &= \left(\int_0^1 a_1(\phi_1'')^2 dx \right) V_1 + \left(\int_0^1 a_1 \phi_1'' \phi_2'' dx \right) V_2 \\
 &= \left(\int_{I_1} a_1(\phi_1'')^2 dx \right) V_1 + \left(\int_{I_2} a_1(\phi_1'')^2 dx \right) V_1 + \left(\int_{I_2} a_1 \phi_1'' \phi_2'' dx \right) V_2 \\
 &= \frac{6}{h^3} (2V_1 - V_2) \\
 A_{1,2} &= \sum_{j=1}^n \left(\int_0^1 a_2 \phi_j'' \phi_1'' dx \right) V_j \\
 &= \left(\int_0^1 a_2(\phi_1'')^2 dx \right) V_1 + \left(\int_0^1 a_2 \phi_1'' \phi_2'' dx \right) V_2 \\
 &= \left(\int_{I_2} a_2(\phi_1'')^2 dx \right) V_1 + \left(\int_{I_2} a_2 \phi_1'' \phi_2'' dx \right) V_2 \\
 &= \frac{6}{h^3} (V_1 - V_2) \\
 A_{2,1} &= \sum_{j=1}^n \left(\int_0^1 a_1 \phi_j'' \phi_2'' dx \right) V_j \\
 &= \left(\int_0^1 a_1 \phi_1'' \phi_2'' dx \right) V_1 + \left(\int_0^1 a_1(\phi_2'')^2 dx \right) V_2 \\
 &= \left(\int_{I_2} a_1 \phi_1'' \phi_2'' dx \right) V_1 + \left(\int_{I_2} a_1(\phi_2'')^2 dx \right) V_2 \\
 &= \frac{6}{h^3} (-V_1 + V_2) \\
 A_{2,2} &= \sum_{j=1}^n \left(\int_0^1 a_2 \phi_j'' \phi_2'' dx \right) V_j \\
 &= \left(\int_0^1 a_2 \phi_1'' \phi_2'' dx \right) V_1 + \left(\int_0^1 a_2(\phi_2'')^2 dx \right) V_2 + \left(\int_0^1 a_2 \phi_2'' \phi_3'' dx \right) V_3 \\
 &= \left(\int_{I_2} a_2 \phi_1'' \phi_2'' dx \right) V_1 + \left(\int_{I_2} a_2(\phi_2'')^2 dx \right) V_2 + \left(\int_{I_3} a_2(\phi_2'')^2 dx \right) V_2 + \left(\int_{I_3} a_2 \phi_2'' \phi_3'' dx \right) V_3
 \end{aligned}$$

$$= \frac{6}{h^3}(-V_1 + 2V_2 - V_3)$$

$$\begin{aligned} A_{2,3} &= \sum_{j=1}^n \left(\int_0^1 a_3 \phi_j'' \phi_2'' dx \right) V_j \\ &= \left(\int_0^1 a_3 (\phi_2'')^2 dx \right) V_2 + \left(\int_0^1 a_3 \phi_2'' \phi_3'' dx \right) V_3 \\ &= \left(\int_{I_3} a_3 (\phi_2'')^2 dx \right) V_2 + \left(\int_{I_3} a_3 \phi_2'' \phi_3'' dx \right) V_3 \\ &= \frac{6}{h^3}(V_2 - V_3) \end{aligned}$$

$$A = \frac{6}{h^3} \begin{pmatrix} V_1 & 2V_1 - V_2 & V_1 - V_2 & 0 & 0 & \cdots \\ 0 & -V_1 + V_2 & -V_1 + 2V_2 - V_3 & V_2 - V_3 & 0 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \cdots & 0 & -V_{n-2} + V_{n-1} & -V_{n-2} + 2V_{n-1} - V_n & V_{n-1} - V_n & 0 \\ \cdots & 0 & 0 & -V_{n-1} + V_n & -V_{n-1} + 2V_n & V_n \end{pmatrix}$$

$$B_{i,k} = \sum_{j=1}^n \left(\int_0^1 a_k \psi_j'' \phi_i'' dx \right) V_j'$$

$$\begin{aligned} B_{1,0} &= \sum_{j=1}^n \left(\int_0^1 a_0 \psi_j'' \phi_1'' dx \right) V_j' \\ &= \left(\int_0^1 a_0 \psi_1'' \phi_1'' dx \right) V_1' \\ &= \left(\int_{I_1} a_0 \psi_1'' \phi_1'' dx \right) V_1' \\ &= -\frac{2}{h^2} V_1' \end{aligned}$$

$$\begin{aligned} B_{1,1} &= \sum_{j=1}^n \left(\int_0^1 a_1 \psi_j'' \phi_1'' dx \right) V_j' \\ &= \left(\int_0^1 a_1 \psi_1'' \phi_1'' dx \right) V_1' + \left(\int_0^1 a_1 \psi_2'' \phi_1'' dx \right) V_2' \\ &= \left(\int_{I_1} a_1 \psi_1'' \phi_1'' dx \right) V_1' + \left(\int_{I_2} a_1 \psi_1'' \phi_1'' dx \right) V_1' + \left(\int_{I_2} a_1 \psi_2'' \phi_1'' dx \right) V_2' \\ &= \frac{2}{h^2} V_2' \end{aligned}$$

$$\begin{aligned}
 B_{1,2} &= \sum_{j=1}^n \left(\int_0^1 a_2 \psi_j'' \phi_1'' dx \right) V_j' \\
 &= \left(\int_0^1 a_2 \psi_1'' \phi_1'' dx \right) V_1' + \left(\int_0^1 a_2 \psi_2'' \phi_1'' dx \right) V_2' \\
 &= \left(\int_{I_2} a_2 \psi_1'' \phi_1'' dx \right) V_1' + \left(\int_{I_2} a_2 \psi_2'' \phi_1'' dx \right) V_2' \\
 &= \frac{2}{h^2} (V_1' + 2V_2')
 \end{aligned}$$

$$\begin{aligned}
 B_{2,1} &= \sum_{j=1}^n \left(\int_0^1 a_1 \psi_j'' \phi_2'' dx \right) V_j' \\
 &= \left(\int_0^1 a_1 \psi_1'' \phi_2'' dx \right) V_1' + \left(\int_0^1 a_1 \psi_2'' \phi_2'' dx \right) V_2' \\
 &= \left(\int_{I_2} a_1 \psi_1'' \phi_2'' dx \right) V_1' + \left(\int_{I_2} a_1 \psi_2'' \phi_2'' dx \right) V_2' \\
 &= \frac{2}{h^2} (-2V_1' - V_2')
 \end{aligned}$$

$$\begin{aligned}
 B_{2,2} &= \sum_{j=1}^n \left(\int_0^1 a_2 \psi_j'' \phi_2'' dx \right) V_j' \\
 &= \left(\int_0^1 a_2 \psi_1'' \phi_2'' dx \right) V_1' + \left(\int_0^1 a_2 \psi_2'' \phi_2'' dx \right) V_2' + \left(\int_0^1 a_2 \psi_3'' \phi_2'' dx \right) V_3' \\
 &= \left(\int_{I_2} a_2 \psi_1'' \phi_2'' dx \right) V_1' + \left(\int_{I_2} a_2 \psi_2'' \phi_2'' dx \right) V_2' + \left(\int_{I_3} a_2 \psi_2'' \phi_2'' dx \right) V_2' + \left(\int_{I_3} a_2 \psi_3'' \phi_2'' dx \right) V_3' \\
 &= \frac{2}{h^2} (-V_1' + V_3')
 \end{aligned}$$

$$\begin{aligned}
 B_{2,3} &= \sum_{j=1}^n \left(\int_0^1 a_3 \psi_j'' \phi_2'' dx \right) V_j' \\
 &= \left(\int_0^1 a_3 \psi_2'' \phi_2'' dx \right) V_2' + \left(\int_0^1 a_3 \psi_3'' \phi_2'' dx \right) V_3' \\
 &= \left(\int_{I_3} a_3 \psi_2'' \phi_2'' dx \right) V_2' + \left(\int_{I_3} a_3 \psi_3'' \phi_2'' dx \right) V_3' \\
 &= \frac{2}{h^2} (V_2' + 2V_3')
 \end{aligned}$$

$$B = \frac{2}{h^2} \begin{pmatrix} -V'_1 & V'_2 & V'_1 + 2V'_2 & 0 & 0 & \cdots \\ 0 & -2V'_1 - V'_2 & -V'_1 + V'_3 & V'_2 + 2V'_3 & 0 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \cdots & 0 & -2V'_{n-2} - V'_{n-1} & -V'_{n-2} + V'_n & V'_{n-1} + 2V'_n & 0 \\ \cdots & 0 & 0 & -2V'_{n-1} - V'_n & -V'_{n-1} & V'_n \end{pmatrix}$$

$$G_{i,k} = \sum_{j=1}^n \left(\int_0^1 a_k \phi_j'' \psi_i'' dx \right) V_j$$

$$\begin{aligned} G_{1,0} &= \sum_{j=1}^n \left(\int_0^1 a_0 \phi_j'' \psi_1'' dx \right) V_j \\ &= \left(\int_0^1 a_0 \phi_1'' \psi_1'' dx \right) V_1 \\ &= \left(\int_{I_1} a_0 \phi_1'' \psi_1'' dx \right) V_1 \\ &= -\frac{2}{h^2} V_1 \end{aligned}$$

$$\begin{aligned} G_{1,1} &= \sum_{j=1}^n \left(\int_0^1 a_1 \phi_j'' \psi_1'' dx \right) V_j \\ &= \left(\int_0^1 a_1 \phi_1'' \psi_1'' dx \right) V_1 + \left(\int_0^1 a_1 \phi_2'' \psi_1'' dx \right) V_2 \\ &= \left(\int_{I_1} a_1 \phi_1'' \psi_1'' dx \right) V_1 + \left(\int_{I_2} a_1 \phi_1'' \psi_1'' dx \right) V_1 + \left(\int_{I_2} a_1 \phi_2'' \psi_1'' dx \right) V_2 \\ &= -\frac{4}{h^2} V_2 \end{aligned}$$

$$\begin{aligned} G_{1,2} &= \sum_{j=1}^n \left(\int_0^1 a_2 \phi_j'' \psi_1'' dx \right) V_j \\ &= \left(\int_0^1 a_2 \phi_1'' \psi_1'' dx \right) V_1 + \left(\int_0^1 a_2 \phi_2'' \psi_1'' dx \right) V_2 \\ &= \left(\int_{I_2} a_2 \phi_1'' \psi_1'' dx \right) V_1 + \left(\int_{I_2} a_2 \phi_2'' \psi_1'' dx \right) V_2 \\ &= \frac{2}{h^2} (V_1 - V_2) \end{aligned}$$

$$G_{2,1} = \sum_{j=1}^n \left(\int_0^1 a_1 \phi_j'' \psi_2'' dx \right) V_j$$

$$\begin{aligned}
 &= \left(\int_0^1 a_1 \phi_1'' \psi_2'' dx \right) V_1 + \left(\int_0^1 a_1 \phi_2'' \psi_2'' dx \right) V_2 \\
 &= \left(\int_{I_2} a_1 \phi_1'' \psi_2'' dx \right) V_1 + \left(\int_{I_2} a_1 \phi_2'' \psi_2'' dx \right) V_2 \\
 &= \frac{2}{h^2} (V_1 - V_2)
 \end{aligned}$$

$$\begin{aligned}
 G_{2,2} &= \sum_{j=1}^n \left(\int_0^1 a_2 \phi_j'' \psi_2'' dx \right) V_j \\
 &= \left(\int_0^1 a_2 \phi_1'' \psi_2'' dx \right) V_1 + \left(\int_0^1 a_2 \phi_2'' \psi_2'' dx \right) V_2 + \left(\int_0^1 a_2 \phi_3'' \psi_2'' dx \right) V_3 \\
 &= \left(\int_{I_2} a_2 \phi_1'' \psi_2'' dx \right) V_1 + \left(\int_{I_2} a_2 \phi_2'' \psi_2'' dx \right) V_2 + \left(\int_{I_3} a_2 \phi_2'' \psi_2'' dx \right) V_2 + \left(\int_{I_3} a_2 \phi_3'' \psi_2'' dx \right) V_3 \\
 &= \frac{2}{h^2} (2V_1 - 2V_3)
 \end{aligned}$$

$$\begin{aligned}
 G_{2,3} &= \sum_{j=1}^n \left(\int_0^1 a_3 \phi_j'' \psi_2'' dx \right) V_j \\
 &= \left(\int_0^1 a_3 \phi_2'' \psi_2'' dx \right) V_2 + \left(\int_0^1 a_3 \phi_3'' \psi_2'' dx \right) V_3 \\
 &= \left(\int_{I_3} a_3 \phi_2'' \psi_2'' dx \right) V_2 + \left(\int_{I_3} a_3 \phi_3'' \psi_2'' dx \right) V_3 \\
 &= \frac{2}{h^2} (V_2 - V_3)
 \end{aligned}$$

$$G = \frac{2}{h^2} \begin{pmatrix} -V_1 & -2V_2 & V_1 - V_2 & 0 & 0 & \cdots \\ 0 & V_1 - V_2 & 2V_1 - 2V_3 & V_2 - V_3 & 0 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \cdots & 0 & V_{n-2} - V_{n-1} & 2V_{n-2} - 2V_n & V_{n-1} - V_n & 0 \\ \cdots & 0 & 0 & V_{n-1} - V_n & 2V_{n-1} & V_n \end{pmatrix}$$

$$H_{i,k} = \sum_{j=1}^n \left(\int_0^1 a_k \psi_j'' \psi_i'' dx \right) V_j'$$

$$\begin{aligned}
 H_{1,0} &= \sum_{j=1}^n \left(\int_0^1 a_0 \psi_j'' \psi_1'' dx \right) V_j' \\
 &= \left(\int_0^1 a_0 (\psi_1'')^2 dx \right) V_1'
 \end{aligned}$$

$$\begin{aligned}
 &= \left(\int_0^1 I_1 a_0 (\psi_1'')^2 dx \right) V_1' \\
 &= \frac{1}{h} V_1' \\
 H_{1,1} &= \sum_{j=1}^n \left(\int_0^1 a_1 \psi_j'' \psi_1'' dx \right) V_j' \\
 &= \left(\int_0^1 a_1 (\psi_1'')^2 dx \right) V_1' + \left(\int_0^1 a_1 \psi_1'' \psi_2'' dx \right) V_2' \\
 &= \left(\int_{I_1} a_1 (\psi_1'')^2 dx \right) V_1' + \left(\int_{I_2} a_1 (\psi_1'')^2 dx \right) V_1' + \left(\int_{I_2} a_1 \psi_1'' \psi_2'' dx \right) V_2' \\
 &= \frac{1}{h} (6V_1' + V_2') \\
 H_{1,2} &= \sum_{j=1}^n \left(\int_0^1 a_2 \psi_j'' \psi_1'' dx \right) V_j' \\
 &= \left(\int_0^1 a_2 (\psi_1'')^2 dx \right) V_1' + \left(\int_0^1 a_2 \psi_1'' \psi_2'' dx \right) V_2' \\
 &= \left(\int_{I_2} a_2 (\psi_1'')^2 dx \right) V_1' + \left(\int_{I_2} a_2 \psi_1'' \psi_2'' dx \right) V_2' \\
 &= \frac{1}{h} (V_1' + V_2') \\
 H_{2,1} &= \sum_{j=1}^n \left(\int_0^1 a_1 \psi_j'' \psi_2'' dx \right) V_j' \\
 &= \left(\int_0^1 a_1 \psi_1'' \psi_2'' dx \right) V_1' + \left(\int_0^1 a_1 (\psi_2'')^2 dx \right) V_2' \\
 &= \left(\int_{I_2} a_1 \psi_1'' \psi_2'' dx \right) V_1' + \left(\int_{I_2} a_1 (\psi_2'')^2 dx \right) V_2' \\
 &= \frac{1}{h} (V_1' + V_2') \\
 H_{2,2} &= \sum_{j=1}^n \left(\int_0^1 a_2 \psi_j'' \psi_2'' dx \right) V_j' \\
 &= \left(\int_0^1 a_2 \psi_1'' \psi_2'' dx \right) V_1' + \left(\int_0^1 a_2 (\psi_2'')^2 dx \right) V_2' + \left(\int_0^1 a_2 \psi_2'' \psi_3'' dx \right) V_3' \\
 &= \left(\int_{I_2} a_2 \psi_1'' \psi_2'' dx \right) V_1' + \left(\int_{I_2} a_2 (\psi_2'')^2 dx \right) V_2' + \left(\int_{I_3} a_2 (\psi_2'')^2 dx \right) V_2' + \left(\int_{I_3} a_2 \psi_2'' \psi_3'' dx \right) V_3' \\
 &= \frac{1}{h} (V_1' + 6V_2' + V_3')
 \end{aligned}$$

$$\begin{aligned}
 H_{2,3} &= \sum_{j=1}^n \left(\int_0^1 a_3 \psi_j'' \psi_2'' dx \right) V_j' \\
 &= \left(\int_0^1 a_3 (\psi_2'')^2 dx \right) V_2' + \left(\int_0^1 a_3 \psi_2'' \psi_3'' dx \right) V_3' \\
 &= \left(\int_{I_3} a_3 (\psi_2'')^2 dx \right) V_2' + \left(\int_{I_3} a_3 \psi_2'' \psi_3'' dx \right) V_3' \\
 &= \frac{1}{h} (V_2' + V_3')
 \end{aligned}$$

$$H = \frac{1}{h} \begin{pmatrix} V_1' & 6V_1' + V_2' & V_1' + V_2' & 0 & 0 & \cdots \\ 0 & V_1' + V_2' & V_1' + 6V_2' + V_3' & V_2' + V_3' & 0 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \cdots & 0 & V_{n-2}' + V_{n-1}' & V_{n-2}' + 6V_{n-1}' + V_n' & V_{n-1}' + V_n' & 0 \\ \cdots & 0 & 0 & V_{n-1}' + V_n' & V_{n-1}' + 6V_n' & V_n' \end{pmatrix}$$

$$C_{i,k} = \sum_{j=1}^n \left(\int_0^1 b_k \phi_j' \phi_i' dx \right) V_j$$

$$\begin{aligned}
 C_{1,0} &= \sum_{j=1}^n \left(\int_0^1 b_0 \phi_j' \phi_1' dx \right) V_j \\
 &= \left(\int_{I_1} b_0 (\phi_1')^2 dx \right) V_1 \\
 &= V_1 \frac{h}{6} [b_0(x_0) \phi_1'(x_0)^2 + 4b_0(x_{1/2}) \phi_1'(x_{1/2})^2 + b_0(x_1) \phi_1'(x_1)^2] \\
 &= V_1 \frac{h}{6} \left[0 + (4) \left(\frac{1}{2} \right) \left(\frac{3}{2h} \right)^2 + 0 \right] \\
 &= \frac{3}{4h} V_1
 \end{aligned}$$

$$\begin{aligned}
 C_{1,1} &= \sum_{j=1}^n \left(\int_0^1 b_1 \phi_j' \phi_1' dx \right) V_j \\
 &= \left(\int_0^1 b_1 (\phi_1')^2 dx \right) V_1 + \left(\int_0^1 b_1 \phi_1' \phi_2' dx \right) V_2 \\
 &= \left(\int_{I_1} b_1 (\phi_1')^2 dx \right) V_1 + \left(\int_{I_2} b_1 (\phi_1')^2 dx \right) V_1 + \left(\int_{I_2} b_1 \phi_1' \phi_2' dx \right) V_2 \\
 &= \frac{3}{4h} (2V_1 - V_2)
 \end{aligned}$$

$$\begin{aligned}
 C_{1,2} &= \sum_{j=1}^n \left(\int_0^1 b_2 \phi'_j \phi'_1 \, dx \right) V_j \\
 &= \left(\int_0^1 b_2 (\phi'_1)^2 \, dx \right) V_1 + \left(\int_0^1 b_2 \phi'_2 \phi'_1 \, dx \right) V_2 \\
 &= \left(\int_{I_2} b_2 (\phi'_1)^2 \, dx \right) V_1 + \left(\int_{I_2} b_2 \phi'_2 \phi'_1 \, dx \right) V_2 \\
 &= \frac{3}{4h} (V_1 - V_2)
 \end{aligned}$$

$$C_{2,0} = 0$$

$$\begin{aligned}
 C_{2,1} &= \sum_{j=1}^n \left(\int_0^1 b_1 \phi'_j \phi'_2 \, dx \right) V_j \\
 &= \left(\int_0^1 b_1 \phi'_1 \phi'_2 \, dx \right) V_1 + \left(\int_0^1 b_1 (\phi'_2)^2 \, dx \right) V_2 \\
 &= \left(\int_{I_2} b_1 \phi'_1 \phi'_2 \, dx \right) V_1 + \left(\int_{I_2} b_1 (\phi'_2)^2 \, dx \right) V_2 \\
 &= \frac{3}{4h} (-V_1 + V_2)
 \end{aligned}$$

$$\begin{aligned}
 C_{2,2} &= \sum_{j=1}^n \left(\int_0^1 b_2 \phi'_j \phi'_2 \, dx \right) V_j \\
 &= \left(\int_0^1 b_2 \phi'_1 \phi'_2 \, dx \right) V_1 + \left(\int_0^1 b_2 (\phi'_2)^2 \, dx \right) V_2 + \left(\int_0^1 b_2 \phi'_3 \phi'_2 \, dx \right) V_3 \\
 &= \left(\int_{I_2} b_2 \phi'_1 \phi'_2 \, dx \right) V_1 + \left(\int_{I_2} b_2 (\phi'_2)^2 \, dx \right) V_2 + \left(\int_{I_3} b_2 (\phi'_2)^2 \, dx \right) V_2 + \left(\int_{I_3} b_2 \phi'_3 \phi'_2 \, dx \right) V_3 \\
 &= \frac{3}{4h} (-V_1 + 2V_2 - V_3)
 \end{aligned}$$

$$\begin{aligned}
 C_{2,3} &= \sum_{j=1}^n \left(\int_0^1 b_3 \phi'_j \phi'_2 \, dx \right) V_j \\
 &= \left(\int_0^1 b_3 (\phi'_2)^2 \, dx \right) V_2 + \left(\int_0^1 b_3 \phi'_3 \phi'_2 \, dx \right) V_3 \\
 &= \left(\int_{I_3} b_3 (\phi'_2)^2 \, dx \right) V_2 + \left(\int_{I_3} b_3 \phi'_3 \phi'_2 \, dx \right) V_3 \\
 &= \frac{3}{4h} (V_2 - V_3)
 \end{aligned}$$

$$C = \frac{3}{4h} \begin{pmatrix} V_1 & 2V_1 - V_2 & V_1 - V_2 & 0 & 0 & \cdots \\ 0 & -V_1 + V_2 & -V_1 + 2V_2 - V_3 & V_2 - V_3 & 0 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \cdots & 0 & -V_{n-2} + V_{n-1} & -V_{n-2} + 2V_{n-1} - V_n & V_{n-1} - V_n & 0 \\ \cdots & 0 & 0 & -V_{n-1} + V_n & -V_{n-1} + 2V_n & V_n \end{pmatrix}$$

$$D_{i,k} = \sum_{j=1}^n \left(\int_0^1 b_k \psi'_j \phi'_i dx \right) V'_j$$

$$\begin{aligned} D_{1,0} &= \sum_{j=1}^n \left(\int_0^1 b_0 \psi'_j \phi'_1 dx \right) V'_j \\ &= \left(\int_0^1 b_0 \psi'_1 \phi'_1 dx \right) V'_1 \\ &= \left(\int_{I_1} b_0 \psi'_1 \phi'_1 dx \right) V'_1 \\ &= -\frac{1}{8} V'_1 \end{aligned}$$

$$\begin{aligned} D_{1,1} &= \sum_{j=1}^n \left(\int_0^1 b_1 \psi'_j \phi'_1 dx \right) V'_j \\ &= \left(\int_0^1 b_1 \psi'_1 \phi'_1 dx \right) V'_1 + \left(\int_0^1 b_1 \psi'_2 \phi'_1 dx \right) V'_2 \\ &= \left(\int_{I_1} b_1 \psi'_1 \phi'_1 dx \right) V'_1 + \left(\int_{I_2} b_1 \psi'_1 \phi'_1 dx \right) V'_1 + \left(\int_{I_2} b_1 \psi'_2 \phi'_1 dx \right) V'_2 \\ &= \frac{1}{8} V'_2 \end{aligned}$$

$$\begin{aligned} D_{1,2} &= \sum_{j=1}^n \left(\int_0^1 b_2 \psi'_j \phi'_1 dx \right) V'_j \\ &= \left(\int_0^1 b_2 \psi'_1 \phi'_1 dx \right) V'_1 + \left(\int_0^1 b_2 \psi'_2 \phi'_1 dx \right) V'_2 \\ &= \left(\int_{I_2} b_2 \psi'_1 \phi'_1 dx \right) V'_1 + \left(\int_{I_2} b_2 \psi'_2 \phi'_1 dx \right) V'_2 \\ &= \frac{1}{8} (V'_1 + V'_2) \end{aligned}$$

$$D_{2,1} = \sum_{j=1}^n \left(\int_0^1 b_1 \psi'_j \phi'_2 dx \right) V'_j$$

$$\begin{aligned}
 &= \left(\int_0^1 b_1 \psi'_1 \phi'_2 \, dx \right) V'_1 + \left(\int_0^1 b_1 \psi'_2 \phi'_2 \, dx \right) V'_2 \\
 &= \left(\int_{I_2} b_1 \psi'_1 \phi'_2 \, dx \right) V'_1 + \left(\int_{I_2} b_1 \psi'_2 \phi'_2 \, dx \right) V'_2 \\
 &= \frac{1}{8}(-V'_1 - V'_2)
 \end{aligned}$$

$$\begin{aligned}
 D_{2,2} &= \sum_{j=1}^n \left(\int_0^1 b_2 \psi'_j \phi'_2 \, dx \right) V'_j \\
 &= \left(\int_0^1 b_2 \psi'_1 \phi'_2 \, dx \right) V'_1 + \left(\int_0^1 b_2 \psi'_2 \phi'_2 \, dx \right) V'_2 + \left(\int_0^1 b_2 \psi'_3 \phi'_2 \, dx \right) V'_3 \\
 &= \left(\int_{I_2} b_2 \psi'_1 \phi'_2 \, dx \right) V'_1 + \left(\int_{I_2} b_2 \psi'_2 \phi'_2 \, dx \right) V'_2 + \left(\int_{I_3} b_2 \psi'_2 \phi'_2 \, dx \right) V'_2 + \left(\int_{I_3} b_2 \psi'_3 \phi'_2 \, dx \right) V'_3 \\
 &= \frac{1}{8}(-V'_1 + V'_3)
 \end{aligned}$$

$$\begin{aligned}
 D_{2,3} &= \sum_{j=1}^n \left(\int_0^1 b_3 \psi'_j \phi'_2 \, dx \right) V'_j \\
 &= \left(\int_0^1 b_3 \psi'_2 \phi'_2 \, dx \right) V'_2 + \left(\int_0^1 b_3 \psi'_3 \phi'_2 \, dx \right) V'_3 \\
 &= \left(\int_{I_3} b_3 \psi'_2 \phi'_2 \, dx \right) V'_2 + \left(\int_{I_3} b_3 \psi'_3 \phi'_2 \, dx \right) V'_3 \\
 &= \frac{1}{8}(V'_2 + V'_3)
 \end{aligned}$$

$$D = \frac{1}{8} \begin{pmatrix} -V'_1 & V'_2 & V'_1 + V'_2 & 0 & 0 & \cdots \\ 0 & -V'_1 - V'_2 & -V'_1 + V'_3 & V'_2 + V'_3 & 0 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \cdots & 0 & -V'_{n-2} - V'_{n-1} & -V'_{n-2} + V'_n & V'_{n-1} + V'_n & 0 \\ \cdots & 0 & 0 & -V'_{n-1} - V'_n & -V'_{n-1} & V'_n \end{pmatrix}$$

$$I_{i,k} = \sum_{j=1}^n \left(\int_0^1 b_k \phi'_j \psi'_i \, dx \right) V'_j$$

$$\begin{aligned}
 I_{1,0} &= \sum_{j=1}^n \left(\int_0^1 b_0 \phi'_j \psi'_1 \, dx \right) V'_j \\
 &= \left(\int_0^1 b_0 \phi'_1 \psi'_1 \, dx \right) V'_1
 \end{aligned}$$

$$\begin{aligned}
 &= \left(\int_{I_1} b_0 \phi'_1 \psi'_1 \, dx \right) V_1 \\
 &= -\frac{1}{8} V_1
 \end{aligned}$$

$$\begin{aligned}
 I_{1,1} &= \sum_{j=1}^n \left(\int_0^1 b_1 \phi'_j \psi'_1 \, dx \right) V_j \\
 &= \left(\int_0^1 b_1 \phi'_1 \psi'_1 \, dx \right) V_1 + \left(\int_0^1 b_1 \phi'_2 \psi'_1 \, dx \right) V_2 \\
 &= \left(\int_{I_1} b_1 \phi'_1 \psi'_1 \, dx \right) V_1 + \left(\int_{I_2} b_1 \phi'_1 \psi'_1 \, dx \right) V_1 + \left(\int_{I_2} b_1 \phi'_2 \psi'_1 \, dx \right) V_2 \\
 &= -\frac{1}{8} V_2
 \end{aligned}$$

$$\begin{aligned}
 I_{1,2} &= \sum_{j=1}^n \left(\int_0^1 b_2 \phi'_j \psi'_1 \, dx \right) V_j \\
 &= \left(\int_0^1 b_2 \phi'_1 \psi'_1 \, dx \right) V_1 + \left(\int_0^1 b_2 \phi'_2 \psi'_1 \, dx \right) V_2 \\
 &= \left(\int_{I_2} b_2 \phi'_1 \psi'_1 \, dx \right) V_1 + \left(\int_{I_2} b_2 \phi'_2 \psi'_1 \, dx \right) V_2 \\
 &= \frac{1}{8} (-V_1 - V_2)
 \end{aligned}$$

$$\begin{aligned}
 I_{2,1} &= \sum_{j=1}^n \left(\int_0^1 b_1 \phi'_j \psi'_2 \, dx \right) V_j \\
 &= \left(\int_0^1 b_1 \phi'_1 \psi'_2 \, dx \right) V_1 + \left(\int_0^1 b_1 \phi'_2 \psi'_2 \, dx \right) V_2 \\
 &= \left(\int_{I_2} b_1 \phi'_1 \psi'_2 \, dx \right) V_1 + \left(\int_{I_2} b_1 \phi'_2 \psi'_2 \, dx \right) V_2 \\
 &= \frac{1}{8} (V_1 - V_2)
 \end{aligned}$$

$$\begin{aligned}
 I_{2,2} &= \sum_{j=1}^n \left(\int_0^1 b_2 \phi'_j \psi'_2 \, dx \right) V_j \\
 &= \left(\int_0^1 b_2 \phi'_1 \psi'_2 \, dx \right) V_1 + \left(\int_0^1 b_2 \phi'_2 \psi'_2 \, dx \right) V_2 + \left(\int_0^1 b_2 \phi'_3 \psi'_2 \, dx \right) V_3 \\
 &= \left(\int_{I_2} b_2 \phi'_1 \psi'_2 \, dx \right) V_1 + \left(\int_{I_2} b_2 \phi'_2 \psi'_2 \, dx \right) V_2 + \left(\int_{I_3} b_2 \phi'_2 \psi'_2 \, dx \right) V_2 + \left(\int_{I_3} b_2 \phi'_3 \psi'_2 \, dx \right) V_3 \\
 &= \frac{1}{8} (V_1 - V_3)
 \end{aligned}$$

$$\begin{aligned}
 I_{2,3} &= \sum_{j=1}^n \left(\int_0^1 b_3 \phi'_j \psi'_2 dx \right) V_j \\
 &= \left(\int_0^1 b_3 \phi'_2 \psi'_2 dx \right) V_2 + \left(\int_0^1 b_3 \phi'_3 \psi'_2 dx \right) V_3 \\
 &= \left(\int_{I_3} b_3 \phi'_2 \psi'_2 dx \right) V_2 + \left(\int_{I_3} b_3 \phi'_3 \psi'_2 dx \right) V_3 \\
 &= \frac{1}{8} (V_2 - V_3)
 \end{aligned}$$

$$I = \frac{1}{8} \begin{pmatrix} -V_1 & -V_2 & V_1 - V_2 & 0 & 0 & \cdots \\ 0 & V_1 - V_2 & V_1 - V_3 & V_2 - V_3 & 0 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \cdots & 0 & V_{n-2} - V_{n-1} & V_{n-2} - V_n & V_{n-1} - V_n & 0 \\ \cdots & 0 & 0 & V_{n-1} - V_n & V_{n-1} & V_n \end{pmatrix}$$

$$J_{i,k} = \sum_{j=1}^n \left(\int_0^1 b_k \psi'_j \psi'_i dx \right) V'_j$$

$$\begin{aligned}
 J_{1,0} &= \sum_{j=1}^n \left(\int_0^1 b_0 \psi'_j \psi'_1 dx \right) V'_j \\
 &= \left(\int_0^1 b_0 \psi'_1 \psi'_1 dx \right) V'_1 \\
 &= \left(\int_{I_1} b_0 \psi'_1 \psi'_1 dx \right) V'_1 \\
 &= \frac{h}{48} V'_1
 \end{aligned}$$

$$\begin{aligned}
 J_{1,1} &= \sum_{j=1}^n \left(\int_0^1 b_1 \psi'_j \psi'_1 dx \right) V'_j \\
 &= \left(\int_0^1 b_1 (\psi'_1)^2 dx \right) V'_1 + \left(\int_0^1 b_1 \psi'_1 \psi'_2 dx \right) V'_2 \\
 &= \left(\int_{I_1} b_1 (\psi'_1)^2 dx \right) V'_1 + \left(\int_{I_2} b_1 (\psi'_1)^2 dx \right) V'_1 + \left(\int_{I_2} b_1 \psi'_1 \psi'_2 dx \right) V'_2 \\
 &= \frac{h}{48} (18V'_1 + V'_2)
 \end{aligned}$$

$$J_{1,2} = \sum_{j=1}^n \left(\int_0^1 b_2 \psi'_j \psi'_1 dx \right) V'_j$$

$$\begin{aligned}
 &= \left(\int_0^1 b_2(\psi'_1)^2 dx \right) V'_1 + \left(\int_0^1 b_2\psi'_1\psi'_2 dx \right) V'_2 \\
 &= \left(\int_{I_2} b_2(\psi'_1)^2 dx \right) V'_1 + \left(\int_{I_2} b_2\psi'_1\psi'_2 dx \right) V'_2 \\
 &= \frac{h}{48}(V'_1 + V'_2)
 \end{aligned}$$

$$\begin{aligned}
 J_{1,2} &= \sum_{j=1}^n \left(\int_0^1 b_2\psi'_j\psi'_1 dx \right) V'_j \\
 &= \left(\int_0^1 b_2(\psi'_1)^2 dx \right) V'_1 + \left(\int_0^1 b_2\psi'_1\psi'_2 dx \right) V'_2 \\
 &= \left(\int_{I_2} b_2(\psi'_1)^2 dx \right) V'_1 + \left(\int_{I_2} b_2\psi'_1\psi'_2 dx \right) V'_2 \\
 &= \frac{h}{48}(V'_1 + V'_2)
 \end{aligned}$$

$$\begin{aligned}
 J_{2,1} &= \sum_{j=1}^n \left(\int_0^1 b_1\psi'_j\psi'_2 dx \right) V'_j \\
 &= \left(\int_0^1 b_1\psi'_1\psi'_2 dx \right) V'_1 + \left(\int_0^1 b_1(\psi'_2)^2 dx \right) V'_2 \\
 &= \left(\int_{I_2} b_1\psi'_1\psi'_2 dx \right) V'_1 + \left(\int_{I_2} b_1(\psi'_2)^2 dx \right) V'_2 \\
 &= \frac{h}{48}(V'_1 + V'_2)
 \end{aligned}$$

$$\begin{aligned}
 J_{2,2} &= \sum_{j=1}^n \left(\int_0^1 b_2\psi'_j\psi'_2 dx \right) V'_j \\
 &= \left(\int_0^1 b_2\psi'_1\psi'_2 dx \right) V'_1 + \left(\int_0^1 b_2(\psi'_2)^2 dx \right) V'_2 + \left(\int_0^1 b_2\psi'_2\psi'_3 dx \right) V'_3 \\
 &= \left(\int_{I_2} b_2\psi'_1\psi'_2 dx \right) V'_1 + \left(\int_{I_2} b_2(\psi'_2)^2 dx \right) V'_2 + \left(\int_{I_3} b_2(\psi'_2)^2 dx \right) V'_2 + \left(\int_{I_3} b_2\psi'_2\psi'_3 dx \right) V'_3 \\
 &= \frac{h}{48}(V'_1 + 18V'_2 + V'_3)
 \end{aligned}$$

$$\begin{aligned}
 J_{2,3} &= \sum_{j=1}^n \left(\int_0^1 b_3\psi'_j\psi'_2 dx \right) V'_j \\
 &= \left(\int_{I_3} b_3(\psi'_2)^2 dx \right) V'_2 + \left(\int_0^1 b_3\psi'_2\psi'_3 dx \right) V'_3 \\
 &= \left(\int_{I_3} b_3(\psi'_2)^2 dx \right) V'_2 + \left(\int_0^1 b_3\psi'_2\psi'_3 dx \right) V'_3
 \end{aligned}$$

$$= \frac{h}{48}(V'_2 + V'_3)$$

$$J = \frac{h}{48} \begin{pmatrix} V'_1 & 18V'_1 + V'_2 & V'_1 + V'_2 & 0 & 0 & \cdots \\ 0 & V'_1 + V'_2 & V'_1 + 18V'_2 + V'_3 & V'_2 + V'_3 & 0 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \cdots & 0 & V'_{n-2} + V'_{n-1} & V'_{n-2} + 18V'_{n-1} + V'_n & V'_{n-1} + V'_n & 0 \\ \cdots & 0 & 0 & V'_n + V'_{n-1} & V'_{n-1} + 18V'_n & V'_n \end{pmatrix}$$

$$E_{i,k} = \sum_{j=1}^n \left(\int_0^1 c_k \phi_j \phi_i \, dx \right) V_j$$

$$\begin{aligned} E_{1,0} &= \sum_{j=1}^n \left(\int_0^1 c_0 \phi_j \phi_1 \, dx \right) V_j \\ &= \left(\int_0^1 c_0 (\phi_1)^2 \, dx \right) V_1 \\ &= \left(\int_{I_1} c_0 (\phi_1)^2 \, dx \right) V_1 \\ &= \frac{h}{12} V_1 \end{aligned}$$

$$\begin{aligned} E_{1,1} &= \sum_{j=1}^n \left(\int_0^1 c_1 \phi_j \phi_1 \, dx \right) V_j \\ &= \left(\int_0^1 c_1 (\phi_1)^2 \, dx \right) V_1 + \left(\int_0^1 c_1 \phi_1 \phi_2 \, dx \right) V_2 \\ &= \left(\int_{I_1} c_1 (\phi_1)^2 \, dx \right) V_1 + \left(\int_{I_2} c_1 (\phi_1)^2 \, dx \right) V_1 + \left(\int_{I_2} c_1 \phi_1 \phi_2 \, dx \right) V_2 \\ &= \frac{h}{12} (6V_1 + V_2) \end{aligned}$$

$$\begin{aligned} E_{1,2} &= \sum_{j=1}^n \left(\int_0^1 c_2 \phi_j \phi_1 \, dx \right) V_j \\ &= \left(\int_0^1 c_2 (\phi_1)^2 \, dx \right) V_1 + \left(\int_0^1 c_2 \phi_1 \phi_2 \, dx \right) V_2 \\ &= \left(\int_{I_2} c_2 (\phi_1)^2 \, dx \right) V_1 + \left(\int_{I_2} c_2 \phi_1 \phi_2 \, dx \right) V_2 \\ &= \frac{h}{12} (V_1 + V_2) \end{aligned}$$

$$\begin{aligned}
 E_{2,1} &= \sum_{j=1}^n \left(\int_0^1 c_1 \phi_j \phi_2 \, dx \right) V_j \\
 &= \left(\int_0^1 c_1 \phi_1 \phi_2 \, dx \right) V_1 + \left(\int_0^1 c_1 (\phi_2)^2 \, dx \right) V_2 \\
 &= \left(\int_{I_2} c_1 \phi_1 \phi_2 \, dx \right) V_1 + \left(\int_{I_2} c_1 (\phi_2)^2 \, dx \right) V_2 \\
 &= \frac{h}{12} (V_1 + V_2)
 \end{aligned}$$

$$\begin{aligned}
 E_{2,2} &= \sum_{j=1}^n \left(\int_0^1 c_2 \phi_j \phi_2 \, dx \right) V_j \\
 &= \left(\int_0^1 c_2 \phi_1 \phi_2 \, dx \right) V_1 + \left(\int_0^1 c_2 (\phi_2)^2 \, dx \right) V_2 + \left(\int_0^1 c_2 \phi_2 \phi_3 \, dx \right) V_3 \\
 &= \left(\int_{I_2} c_2 \phi_1 \phi_2' \, dx \right) V_1 + \left(\int_{I_2} c_2 (\phi_2)^2 \, dx \right) V_2 + \left(\int_{I_3} c_2 (\phi_2)^2 \, dx \right) V_2 + \left(\int_{I_3} c_2 \phi_2 \phi_3 \, dx \right) V_3 \\
 &= \frac{h}{12} (V_1 + 6V_2 + V_3)
 \end{aligned}$$

$$\begin{aligned}
 E_{2,3} &= \sum_{j=1}^n \left(\int_0^1 c_3 \phi_j \phi_2 \, dx \right) V_j \\
 &= \left(\int_0^1 c_3 (\phi_2)^2 \, dx \right) V_2 + \left(\int_0^1 c_3 \phi_2 \phi_3 \, dx \right) V_3 \\
 &= \left(\int_{I_3} c_3 (\phi_2)^2 \, dx \right) V_2 + \left(\int_{I_3} c_3 \phi_2 \phi_3 \, dx \right) V_3 \\
 &= \frac{h}{12} (V_2 + V_3)
 \end{aligned}$$

$$E = \frac{h}{12} \begin{pmatrix} V_1 & 6V_1 + V_2 & V_1 + V_2 & 0 & 0 & \cdots \\ 0 & V_1 + V_2 & V_1 + 6V_2 + V_3 & V_2 + V_3 & 0 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \cdots & 0 & V_{n-2} + V_{n-1} & V_{n-2} + 6V_{n-1} + V_n & V_{n-1} + V_n & 0 \\ \cdots & 0 & 0 & V_n + V_{n-1} & V_{n-1} + 6V_n & V_n \end{pmatrix}$$

$$F_{i,k} = \sum_{j=1}^n \left(\int_0^1 c_k \psi_j \phi_i \, dx \right) V_j'$$

$$F_{1,0} = \sum_{j=1}^n \left(\int_0^1 c_0 \psi_j \phi_1 \, dx \right) V_j'$$

$$\begin{aligned}
 &= \left(\int_0^1 c_0 \psi_1 \phi_1 \, dx \right) V_1' \\
 &= \left(\int_{I_1} c_0 \psi_1 \phi_1 \, dx \right) V_1' \\
 &= -\frac{h^2}{48} V_1'
 \end{aligned}$$

$$\begin{aligned}
 F_{1,1} &= \sum_{j=1}^n \left(\int_0^1 c_1 \psi_j \phi_1 \, dx \right) V_j' \\
 &= \left(\int_0^1 c_1 \psi_1 \phi_1 \, dx \right) V_1' + \left(\int_0^1 c_1 \psi_2 \phi_1 \, dx \right) V_2' \\
 &= \left(\int_{I_1} c_1 \psi_1 \phi_1 \, dx \right) V_1' + \left(\int_{I_2} c_1 \psi_1 \phi_1 \, dx \right) V_1' + \left(\int_{I_2} c_1 \psi_2 \phi_1 \, dx \right) V_2' \\
 &= -\frac{h^2}{48} V_2'
 \end{aligned}$$

$$\begin{aligned}
 F_{1,2} &= \sum_{j=1}^n \left(\int_0^1 c_2 \psi_j \phi_1 \, dx \right) V_j' \\
 &= \left(\int_0^1 c_2 \psi_1 \phi_1 \, dx \right) V_1' + \left(\int_0^1 c_2 \psi_2 \phi_1 \, dx \right) V_2' \\
 &= \left(\int_{I_2} c_2 \psi_1 \phi_1 \, dx \right) V_1' + \left(\int_{I_2} c_2 \psi_2 \phi_1 \, dx \right) V_2' \\
 &= \frac{h^2}{48} (V_1' - V_2')
 \end{aligned}$$

$$\begin{aligned}
 F_{2,1} &= \sum_{j=1}^n \left(\int_0^1 c_1 \psi_j \phi_2 \, dx \right) V_j' \\
 &= \left(\int_0^1 c_1 \psi_1 \phi_2 \, dx \right) V_1' + \left(\int_0^1 c_1 \psi_2 \phi_2 \, dx \right) V_2' \\
 &= \left(\int_{I_2} c_1 \psi_1 \phi_2 \, dx \right) V_1' + \left(\int_{I_2} c_1 \psi_2 \phi_2 \, dx \right) V_2' \\
 &= \frac{h^2}{48} (V_1' - V_2')
 \end{aligned}$$

$$\begin{aligned}
 F_{2,2} &= \sum_{j=1}^n \left(\int_0^1 c_2 \psi_j \phi_2 \, dx \right) V_j' \\
 &= \left(\int_0^1 c_2 \psi_1 \phi_2 \, dx \right) V_1' + \left(\int_0^1 c_2 \psi_2 \phi_2 \, dx \right) V_2' + \left(\int_0^1 c_2 \psi_3 \phi_2 \, dx \right) V_3'
 \end{aligned}$$

$$\begin{aligned}
 &= \left(\int_{I_2} c_2 \psi_1 \phi_2 \, dx \right) V_1' + \left(\int_{I_2} c_2 \psi_2 \phi_2 \, dx \right) V_2' + \left(\int_{I_3} c_2 \psi_2 \phi_2 \, dx \right) V_2' + \left(\int_{I_3} c_2 \psi_3 \phi_2 \, dx \right) V_3' \\
 &= \frac{h^2}{48} (V_1' + V_3')
 \end{aligned}$$

$$\begin{aligned}
 F_{2,3} &= \sum_{j=1}^n \left(\int_0^1 c_3 \psi_j \phi_2 \, dx \right) V_j' \\
 &= \left(\int_0^1 c_3 \psi_2 \phi_2 \, dx \right) V_2' + \left(\int_0^1 c_3 \psi_3 \phi_2 \, dx \right) V_3' \\
 &= \left(\int_{I_3} c_3 \psi_2 \phi_2 \, dx \right) V_2' + \left(\int_{I_3} c_3 \psi_3 \phi_2 \, dx \right) V_3' \\
 &= \frac{h^2}{48} (V_2' - V_3')
 \end{aligned}$$

$$F = \frac{h^2}{48} \begin{pmatrix} -V_1' & -V_2' & V_1' - V_2' & 0 & 0 & \cdots \\ 0 & V_1' - V_2' & V_1' - V_3' & V_2' - V_3' & 0 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \cdots & 0 & V_{n-2}' - V_{n-1}' & V_{n-2}' - V_n' & V_{n-1}' - V_n' & 0 \\ \cdots & 0 & 0 & V_{n-1}' - V_n' & V_{n-1}' & V_n' \end{pmatrix}$$

$$K_{i,k} = \sum_{j=1}^n \left(\int_0^1 c_k \phi_j \psi_i \, dx \right) V_j$$

$$\begin{aligned}
 K_{1,0} &= \sum_{j=1}^n \left(\int_0^1 c_0 \phi_j \psi_1 \, dx \right) V_j \\
 &= \left(\int_0^1 c_0 \phi_1 \psi_1 \, dx \right) V_1 \\
 &= \left(\int_{I_1} c_0 \phi_1 \psi_1 \, dx \right) V_1 \\
 &= -\frac{h^2}{48} V_1
 \end{aligned}$$

$$\begin{aligned}
 K_{1,1} &= \sum_{j=1}^n \left(\int_0^1 c_1 \phi_j \psi_1 \, dx \right) V_j \\
 &= \left(\int_0^1 c_1 \phi_1 \psi_1 \, dx \right) V_1 + \left(\int_0^1 c_1 \phi_2 \psi_1 \, dx \right) V_2 \\
 &= \left(\int_{I_1} c_1 \phi_1 \psi_1 \, dx \right) V_1 + \left(\int_{I_2} c_1 \phi_1 \psi_1 \, dx \right) V_1 + \left(\int_{I_2} c_1 \phi_2 \psi_1 \, dx \right) V_2
 \end{aligned}$$

$$= \frac{h^2}{48} V_2$$

$$\begin{aligned} K_{1,2} &= \sum_{j=1}^n \left(\int_0^1 c_2 \phi_j \psi_1 \, dx \right) V_j \\ &= \left(\int_0^1 c_2 \phi_1 \psi_1 \, dx \right) V_1 + \left(\int_0^1 c_2 \phi_2 \psi_1 \, dx \right) V_2 \\ &= \left(\int_{I_2} c_2 \phi_1 \psi_1 \, dx \right) V_1 + \left(\int_{I_2} c_2 \phi_2 \psi_1 \, dx \right) V_2 \\ &= \frac{h^2}{48} (V_1 + V_2) \end{aligned}$$

$$\begin{aligned} K_{2,1} &= \sum_{j=1}^n \left(\int_0^1 c_1 \phi_j \psi_2 \, dx \right) V_j \\ &= \left(\int_0^1 c_1 \phi_1 \psi_2 \, dx \right) V_1 + \left(\int_0^1 c_1 \phi_2 \psi_2 \, dx \right) V_2 \\ &= \left(\int_{I_2} c_1 \phi_1 \psi_2 \, dx \right) V_1 + \left(\int_{I_2} c_1 \phi_2 \psi_2 \, dx \right) V_2 \\ &= \frac{h^2}{48} (-V_1 - V_2) \end{aligned}$$

$$\begin{aligned} K_{2,2} &= \sum_{j=1}^n \left(\int_0^1 c_2 \phi_j \psi_2 \, dx \right) V_j \\ &= \left(\int_0^1 c_2 \phi_1 \psi_2 \, dx \right) V_1 + \left(\int_0^1 c_2 \phi_2 \psi_2 \, dx \right) V_2 + \left(\int_0^1 c_2 \phi_3 \psi_2 \, dx \right) V_3 \\ &= \left(\int_{I_2} c_2 \phi_1 \psi_2 \, dx \right) V_1 + \left(\int_{I_2} c_2 \phi_2 \psi_2 \, dx \right) V_2 + \left(\int_{I_3} c_2 \phi_2 \psi_2 \, dx \right) V_2 + \left(\int_{I_3} c_2 \phi_3 \psi_2 \, dx \right) V_3 \\ &= \frac{h^2}{48} (-V_1 + V_3) \end{aligned}$$

$$\begin{aligned} K_{2,3} &= \sum_{j=1}^n \left(\int_0^1 c_3 \phi_j \psi_2 \, dx \right) V_j \\ &= \left(\int_0^1 c_3 \phi_2 \psi_2 \, dx \right) V_2 + \left(\int_0^1 c_3 \phi_3 \psi_2 \, dx \right) V_3 \\ &= \left(\int_{I_3} c_3 \phi_2 \psi_2 \, dx \right) V_2 + \left(\int_{I_3} c_3 \phi_3 \psi_2 \, dx \right) V_3 \\ &= \frac{h^2}{48} \end{aligned}$$

$$K = \frac{h^2}{48} \begin{pmatrix} -V_1 & V_2 & V_1 + V_2 & 0 & 0 & \cdots \\ 0 & -V_1 - V_2 & -V_1 + V_3 & V_2 + V_3 & 0 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \cdots & 0 & -V_{n-2} - V_{n-1} & -V_{n-2} + V_n & V_{n-1} + V_n & 0 \\ \cdots & 0 & 0 & -V_n - V_{n-1} & -V_{n-1} & V_n \end{pmatrix}$$

$$L_{i,k} = \sum_{j=1}^n \left(\int_0^1 c_k \psi_j \psi_i \, dx \right) V_j'$$

$$\begin{aligned} L_{1,0} &= \sum_{j=1}^n \left(\int_0^1 c_0 \psi_j \psi_1 \, dx \right) V_j' \\ &= \left(\int_0^1 c_0 (\psi_1)^2 \, dx \right) V_1' \\ &= \left(\int_{I_1} c_0 (\psi_1)^2 \, dx \right) V_1' \\ &= \frac{h^3}{192} V_1' \end{aligned}$$

$$\begin{aligned} L_{1,1} &= \sum_{j=1}^n \left(\int_0^1 c_1 \psi_j \psi_1 \, dx \right) V_j' \\ &= \left(\int_0^1 c_1 (\psi_1)^2 \, dx \right) V_1' + \left(\int_0^1 c_1 \psi_1 \psi_2 \, dx \right) V_2' \\ &= \left(\int_{I_1} c_1 (\psi_1)^2 \, dx \right) V_1' + \left(\int_{I_2} c_1 (\psi_1)^2 \, dx \right) V_1' + \left(\int_{I_2} c_1 \psi_1 \psi_2 \, dx \right) V_2' \\ &= \frac{h^3}{192} (2V_1' - V_2') \end{aligned}$$

$$\begin{aligned} L_{1,2} &= \sum_{j=1}^n \left(\int_0^1 c_2 \psi_j \psi_1 \, dx \right) V_j' \\ &= \left(\int_0^1 c_2 (\psi_1)^2 \, dx \right) V_1' + \left(\int_0^1 c_2 \psi_1 \psi_2 \, dx \right) V_2' \\ &= \left(\int_{I_2} c_2 (\psi_1)^2 \, dx \right) V_1' + \left(\int_{I_2} c_2 \psi_1 \psi_2 \, dx \right) V_2' \\ &= \frac{h^3}{192} (V_1' - V_2') \end{aligned}$$

$$L_{2,1} = \sum_{j=1}^n \left(\int_0^1 c_1 \psi_j \psi_2 \, dx \right) V_j'$$

$$\begin{aligned}
 &= \left(\int_0^1 c_1 \psi_1 \psi_2 \, dx \right) V_1' + \left(\int_0^1 c_1 (\psi_2)^2 \, dx \right) V_2' \\
 &= \left(\int_{I_2} c_1 \psi_1 \psi_2 \, dx \right) V_1' + \left(\int_{I_2} c_1 (\psi_2)^2 \, dx \right) V_2' \\
 &= \frac{h^3}{192} (-V_1' + V_2')
 \end{aligned}$$

$$\begin{aligned}
 L_{2,2} &= \sum_{j=1}^n \left(\int_0^1 c_2 \psi_j \psi_2 \, dx \right) V_j' \\
 &= \left(\int_0^1 c_2 \psi_1 \psi_2 \, dx \right) V_1' + \left(\int_0^1 c_2 (\psi_2)^2 \, dx \right) V_2' + \left(\int_0^1 c_2 \psi_2 \psi_3 \, dx \right) V_3' \\
 &= \left(\int_{I_2} c_2 \psi_1 \psi_2 \, dx \right) V_1' + \left(\int_{I_2} c_2 (\psi_2)^2 \, dx \right) V_2' + \left(\int_{I_3} c_2 (\psi_2)^2 \, dx \right) V_2' + \left(\int_{I_3} c_2 \psi_2 \psi_3 \, dx \right) V_3' \\
 &= \frac{h^3}{192} (-V_1' + 2V_2' - V_3')
 \end{aligned}$$

$$\begin{aligned}
 L_{2,3} &= \sum_{j=1}^n \left(\int_0^1 c_3 \psi_j \psi_2 \, dx \right) V_j' \\
 &= \left(\int_0^1 c_3 (\psi_2)^2 \, dx \right) V_2' + \left(\int_0^1 c_3 \psi_2 \psi_3 \, dx \right) V_3' \\
 &= \left(\int_{I_3} c_3 (\psi_2)^2 \, dx \right) V_2' + \left(\int_{I_3} c_3 \psi_2 \psi_3 \, dx \right) V_3' \\
 &= \frac{h^3}{192} (V_2' - V_3')
 \end{aligned}$$

$$L = \frac{h^3}{192} \begin{pmatrix} V_1' & 2V_1' - V_2' & V_1' - V_2' & 0 & 0 & \cdots \\ 0 & -V_1' + V_2' & -V_1' + 2V_2' - V_3' & V_2' - V_3' & 0 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ \cdots & 0 & -V_{n-2}' + V_{n-1}' & -V_{n-2}' + 2V_{n-1}' - V_n' & V_{n-1}' - V_n' & 0 \\ \cdots & 0 & 0 & V_n' - V_{n-1}' & 2V_n' - V_{n-1}' & V_n' \end{pmatrix}$$

2.4 Output Least-Squares Approach

The output least-squares (OLS) cost functional is discretized by the fourth-order basis functions and formulated as matrix equations. The OLS cost functional is not necessarily guaranteed to be convex and therefore the problem depends heavily on regularization to obtain a unique solution [4].

This is evident in the inaccuracies of the recovered parameter portrayed in the numerical results section.

2.4.1 Discretized Cost Functional

Recall that $q = (a, b, c)$.

$$\begin{aligned}
 J_1(q) &= \frac{1}{2} \|u(q) - z\|_2^2 \\
 &= \frac{1}{2} (u(q) - z, u(q) - z) \\
 &= \frac{1}{2} (\bar{v}, \bar{v}) \\
 &= \frac{1}{2} \left(\sum_{i=1}^n v_i \phi_i + v'_i \psi_i, \sum_{i=1}^n v_i \phi_i + v'_i \right) \\
 &= \frac{1}{2} \int_0^1 \left[\sum_{i=1}^n v_i \phi_i \right] \left[\sum_{i=1}^n v_i \phi_i \right] dx + \frac{1}{2} \int_0^1 2 \left[\sum_{i=1}^n v'_i \psi_i \right] \left[\sum_{i=1}^n v_i \phi_i \right] dx \\
 &\quad + \frac{1}{2} \int_0^1 \left[\sum_{i=1}^n v'_i \psi_i \right] \left[\sum_{i=1}^n v'_i \psi_i \right] dx \\
 &= \frac{1}{2} V^T A V + \frac{1}{2} V^T B V' + \frac{1}{2} V'^T B^T V + \frac{1}{2} V'^T C V' \\
 &= \frac{1}{2} \begin{bmatrix} V & V' \end{bmatrix} \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} \begin{bmatrix} V \\ V' \end{bmatrix} \\
 &= \frac{1}{2} \tilde{V}^T M \tilde{V}
 \end{aligned} \tag{2.32}$$

where $\bar{v} = u(q) - z$, $\tilde{V} = \begin{bmatrix} V \\ V' \end{bmatrix}$, $V = (v_i)_{i=1,2,\dots,n}$, $V' = (v'_i)_{i=1,2,\dots,n}$ and M is the mass matrix derived in (2.10).

2.4.2 Gradient Derivation

First, we rewrite the discretization of the OLS cost functional derived above in an alternate form.

$$J_1(Q) = \frac{1}{2} (U - Z)^T M (U - Z) \tag{2.34}$$

The gradient is now computed utilizing the chain rule of differentiation, the definition of δU in (2.21), and the definition of the adjoint stiffness matrix.

$$\begin{aligned}
 DJ_1(Q)\delta Q &= \frac{1}{2}(\delta U)^T M(U - Z) + \frac{1}{2}(U - Z)^T M(\delta U) \\
 &= (\delta U)^T M(U - Z) \\
 &= [-K(Q)^{-1}K(\delta Q)U]^T M(U - Z) \\
 &= [-K(Q)^{-1}L(U)\delta Q]^T M(U - Z) \\
 &= -(\delta Q)^T L(U)^T (K(Q)^{-1})^T M(U - Z) \\
 &= -(\delta Q)^T L(U)^T K(Q)^{-1} M(U - Z)
 \end{aligned} \tag{2.35}$$

Recall that $Q = (A, B, C)$. Therefore we have that the gradient of (2.34) is

$$\nabla J_1(Q) = -L(U)^T K(Q)^{-1} M(U - Z). \tag{2.36}$$

2.4.3 Direct Problem Numerical Examples

In this section we display numerical solutions to the 1-dimensional fourth-order differential equation on the interval $\Omega = (0, 1)$. In general form, the problem is to solve

$$\frac{d^2}{dx^2} \left(a(x) \frac{d^2}{dx^2} u \right) = f \tag{2.37}$$

$$u(x) = \frac{du}{dx}(x) = 0 \text{ on } \Gamma \tag{2.38}$$

Example 1:

$$u(x) = -\cos(2\pi x) + 1$$

$$a(x) = 1 + x$$

$$f(x) = -16\pi^3 \sin(2\pi x) - 16\pi^4(x + 1) \cos(2\pi x)$$

Example 2:

$$u(x) = -4x^4 + 8x^3 - 4x^2$$

$$a(x) = 1 + x^2$$

$$f(x) = -1440x^2 + 960x - 192$$

Example 3:

$$u(x) = \cos(2\pi x) - 1$$

$$a(x) = 1 + 5(x - 1)x^2$$

$$\begin{aligned} f(x) = & 32\pi^3 \sin(2\pi x)(2x(80x - 80) + 80x^2) - 3840\pi \sin(2\pi x) \\ & + 16\pi^4 \cos(2\pi x)((x^2)(80x - 80) + 1) - 24\pi^2 \cos(2\pi x)(480x - 160) \end{aligned}$$

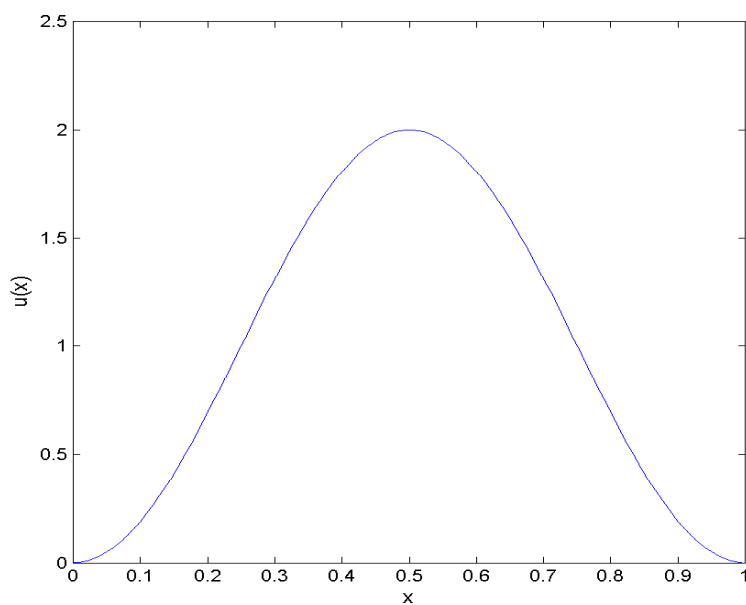


Figure 2.1: Example 1: Direct Problem

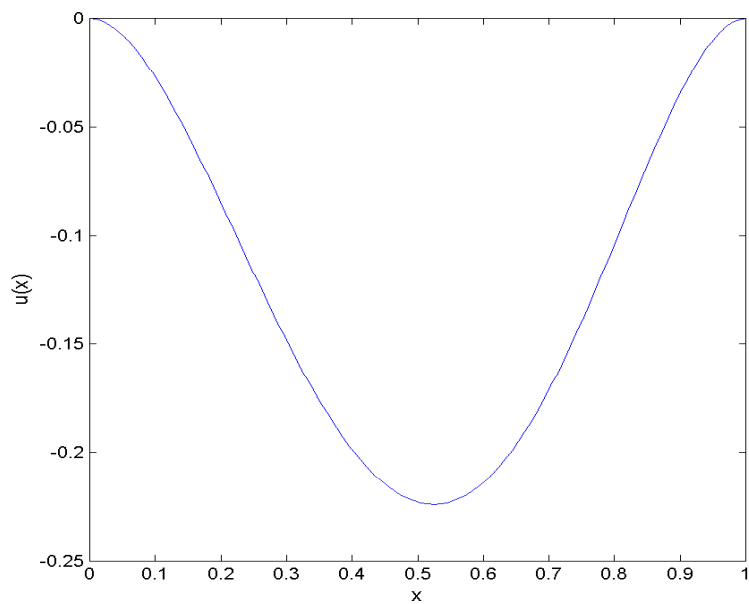


Figure 2.2: Example 2: Direct Problem

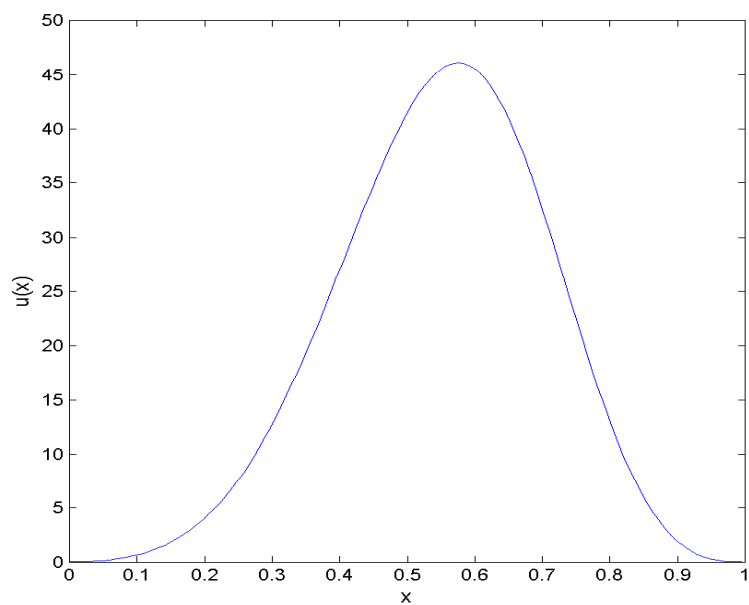


Figure 2.3: Example 3: Direct Problem

We provide numerical examples which involve a fourth-order differential equation containing three

spatially varying coefficients. The coefficient $a(x)$ in the fourth-order term is successfully identified in each example.

2.4.4 Inverse Problem Numerical Examples

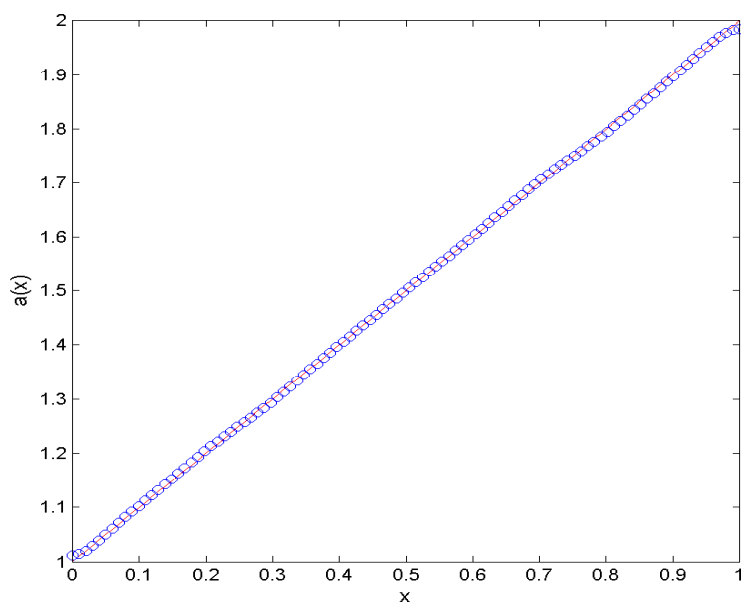


Figure 2.4: Example 1: Inverse Problem

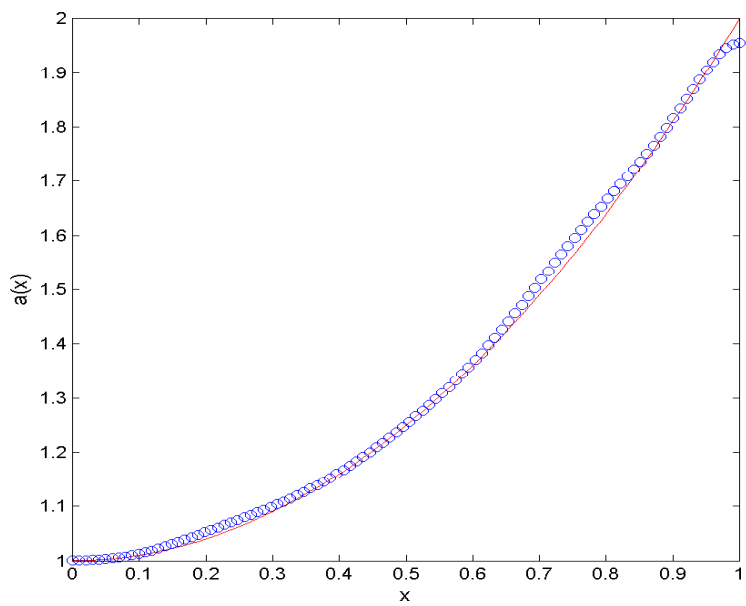


Figure 2.5: Example 2: Inverse Problem

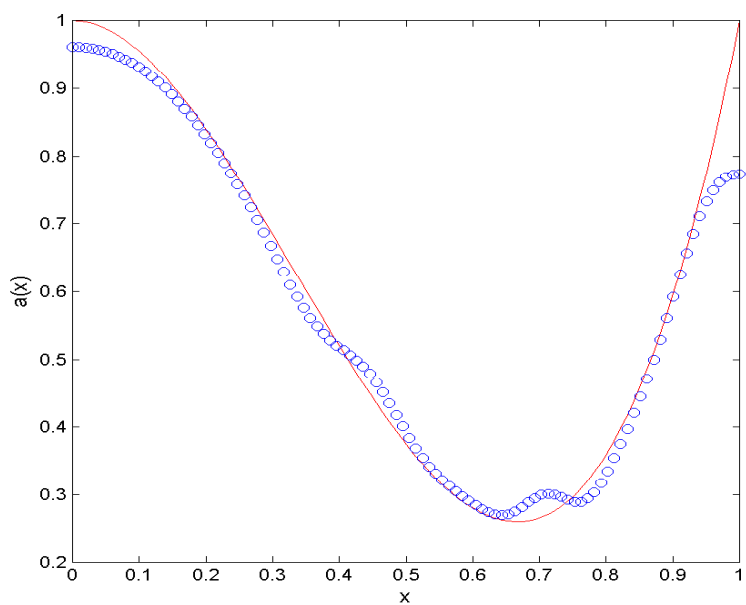


Figure 2.6: Example 3: Inverse Problem

2.5 Modified Output Least-Squares Approach

We derive the discrete modified output-least squares (MOLS) cost functional in the same manner as above. The MOLS cost functional has the advantage over OLS that it is smooth and convex [4]. We see in the numerical results section that the parameter is identified more accurately with MOLS than with OLS.

2.5.1 Discretized Cost Functional

$$\begin{aligned}
 J_2(q) &= \frac{1}{2} T(q, u(q) - z, u(q) - z) \\
 &= \frac{1}{2} \int_0^1 a(x) \left(\frac{d^2 \bar{v}}{dx^2} \right)^2 + b(x) \left(\frac{d \bar{v}}{dx} \right)^2 dx + c(x) \bar{v}^2 \\
 &= \frac{1}{2} \int_0^1 a(x) \left(\sum_{i=1}^n v_i \phi_i'' + v_i' \psi_i'' \right)^2 + b(x) \left(\sum_{i=1}^n v_i \phi_i' + v_i' \psi_i' \right)^2 dx + c(x) \left(\sum_{i=1}^n v_i \phi_i + v_i' \psi_i \right)^2 \\
 &= \frac{1}{2} \begin{bmatrix} V & V' \end{bmatrix} \begin{bmatrix} A + C + E & B + D + F \\ G + I + K & H + J + L \end{bmatrix} \begin{bmatrix} V \\ V' \end{bmatrix} \\
 &= \frac{1}{2} \tilde{V}^T K \tilde{V}
 \end{aligned} \tag{2.39}$$

where $\|\cdot\|_E$ is the energy norm, $\bar{v} = u(a) - z$, and K is the fourth-order stiffness matrix derived in (??).

2.5.2 Gradient Derivation

First, we rewrite the discretization of the MOLS cost functional derived above in an alternate form.

$$J_2(Q) = \frac{1}{2} (U - Z)^T K(Q) (U - Z) \tag{2.41}$$

The gradient is now computed utilizing the chain rule of differentiation, the definition of δU in (2.21), and the definition of the adjoint stiffness matrix.

$$DJ_2(Q)\delta Q = \frac{1}{2}(\delta U)^T K(Q)(U - Z) + \frac{1}{2}(U - Z)^T K(Q)(\delta U) \tag{2.42}$$

$$\begin{aligned}
 & + \frac{1}{2}(U - Z)^T DK(Q)(\delta Q)(U - Z) \\
 & = (\delta U)^T K(Q)(U - Z) + \frac{1}{2}(U - Z)^T K(\delta Q)(U - Z) \\
 & = [-K(Q)^{-1}K(\delta Q)U]^T K(Q)(U - Z) + \frac{1}{2}(U - Z)^T K(\delta Q)(U - Z) \\
 & = -(\delta Q)^T L(U)^T (-K(Q)^{-1})^T K(Q)(U - Z) + \frac{1}{2}(U - Z)^T K(\delta Q)(U - Z) \\
 & = -(\delta Q)^T L(U)^T (U - Z) + \frac{1}{2}(\delta Q)^T L(U - Z)^T (U - Z) \\
 & = -\frac{1}{2}(\delta Q)^T L(U + Z)^T (U - Z)
 \end{aligned}$$

Therefore we have that the gradient of (2.41) is

$$\nabla J_2(Q) = -\frac{1}{2}L(U + Z)^T (U - Z). \quad (2.43)$$

2.5.3 Direct Problem Numerical Examples

Now we display numerical solutions to the 1-dimensional fourth-order differential equation inverse problem solved on the interval $\Omega = (0, 1)$ with the examples provided in 2.4.3 for identifying a single coefficient in the strictly fourth-order system.

In addition to the numerical examples provided in the previous section we display numerical the equations for the examples involving a fourth-order differential equation inverse problem solved on the interval $\Omega = (0, 1)$ for identifying a single coefficient among a three coefficient system. We solve the system represented by

$$\frac{d^2}{dx^2} \left(a(x) \frac{d^2 u(x)}{dx^2} \right) - \frac{d^2}{dx^2} \left(b(x) \frac{d^2 u(x)}{dx^2} \right) + c(x)u(x) = f(x) \quad (2.44)$$

$$u(x) = \frac{du}{dx}(x) = 0 \text{ on } \Gamma \quad (2.45)$$

Example 4:

$$u(x) = x^4 - 2x^3 + x^2$$

$$a(x) = 1 + x^2$$

$$b(x) = 1 + x$$

$$c(x) = 2$$

$$f(x) = 2x^4 + 12x^3 + 140x^2 - 80x + 30$$

Example 5:

$$u(x) = \cos(2\pi x) - 1$$

$$a(x) = 2 + x(x - 1)$$

$$b(x) = 2 + x$$

$$c(x) = 2$$

$$\begin{aligned} f(x) = & 2 \cos(2\pi x) - 2\pi \sin(2\pi x) - 8\pi^2 \cos(2\pi x) - 4\pi^2 \cos(2\pi x)(x + 2) \\ & + 16\pi^4 \cos(2\pi x)(x(x - 1) + 2) + 16\pi^3 \sin(2\pi x)(2x - 1) - 2 \end{aligned}$$

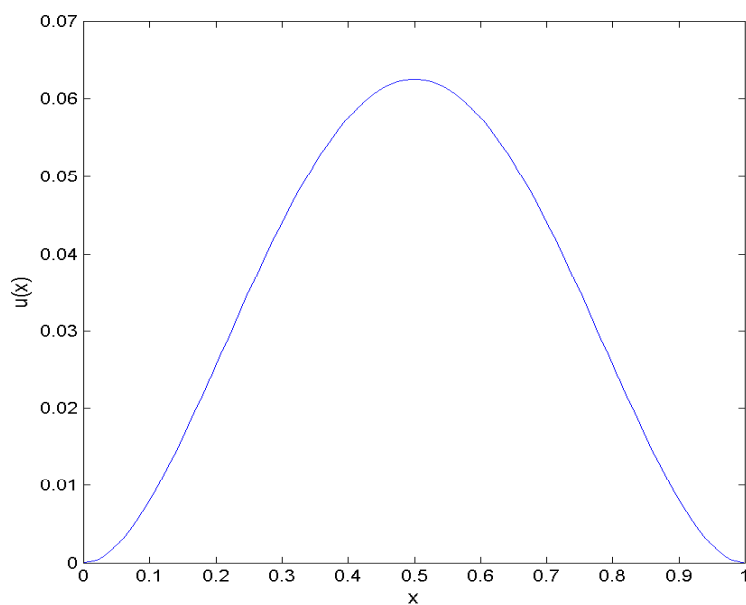


Figure 2.7: Example 4: Direct Problem

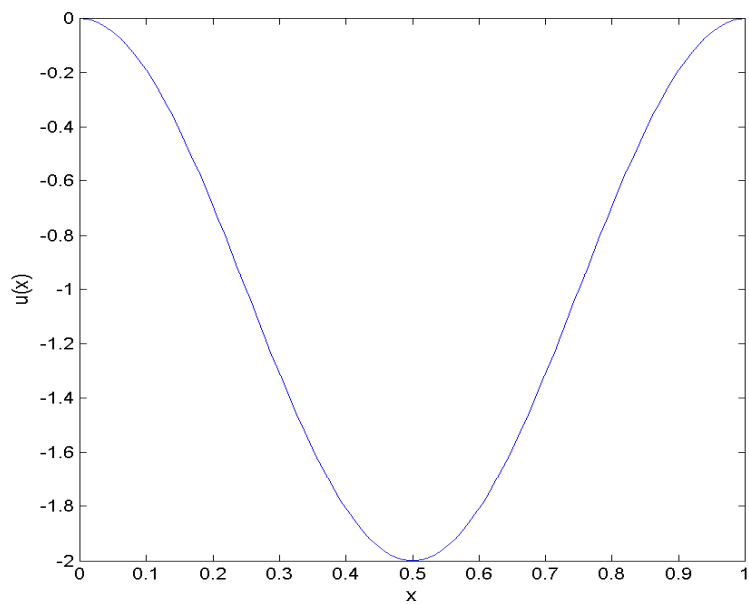


Figure 2.8: Example 5: Direct Problem

2.5.4 Inverse Problem Numerical Examples

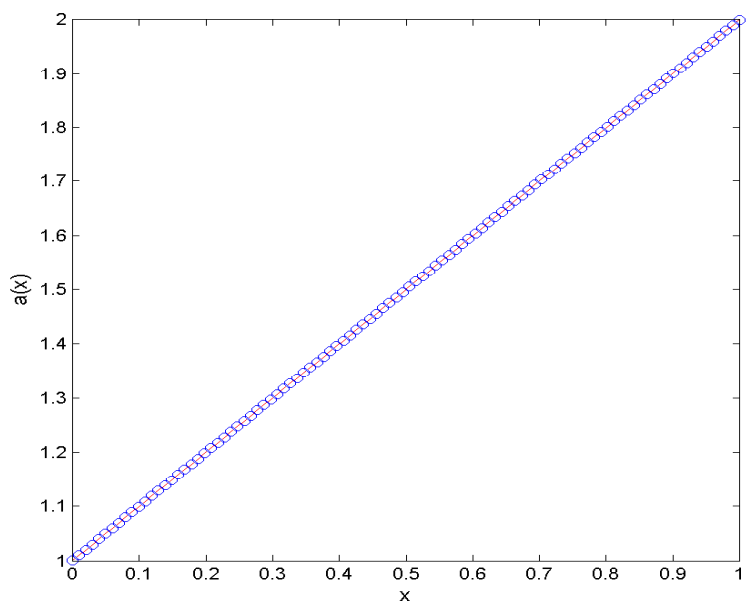


Figure 2.9: Example 1: Inverse Problem

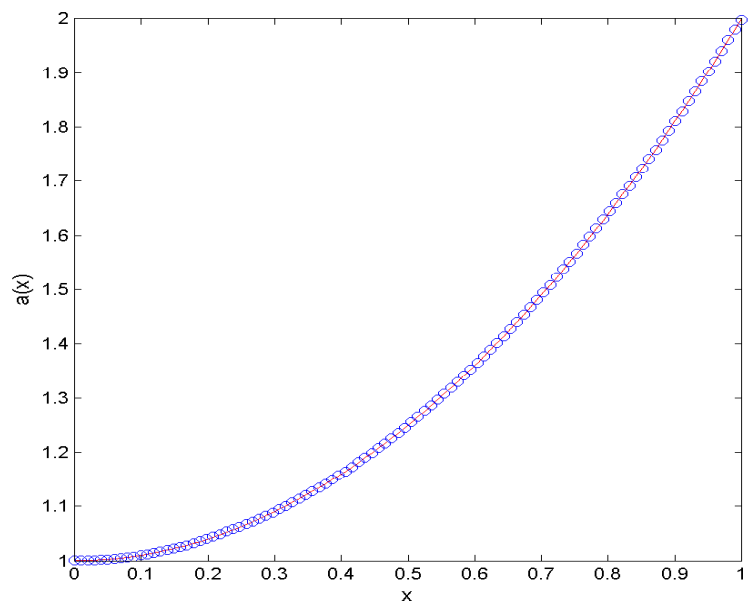


Figure 2.10: Example 2: Inverse Problem

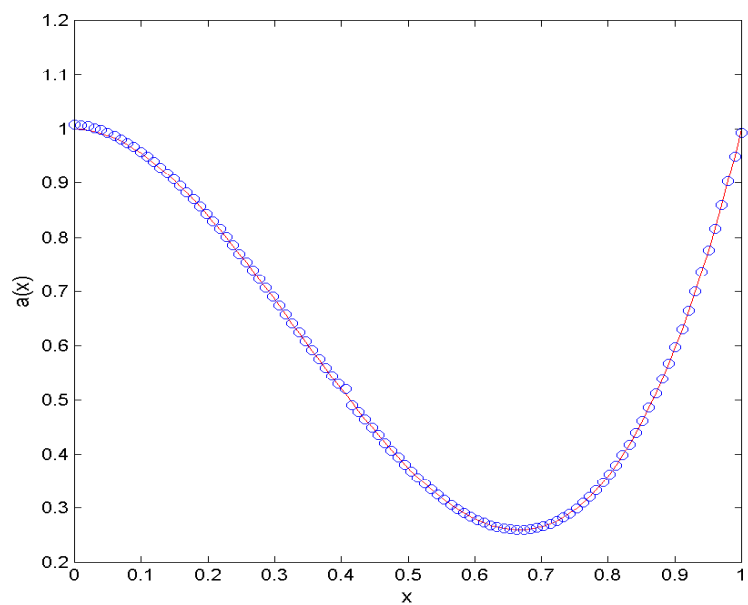


Figure 2.11: Example 3: Inverse Problem

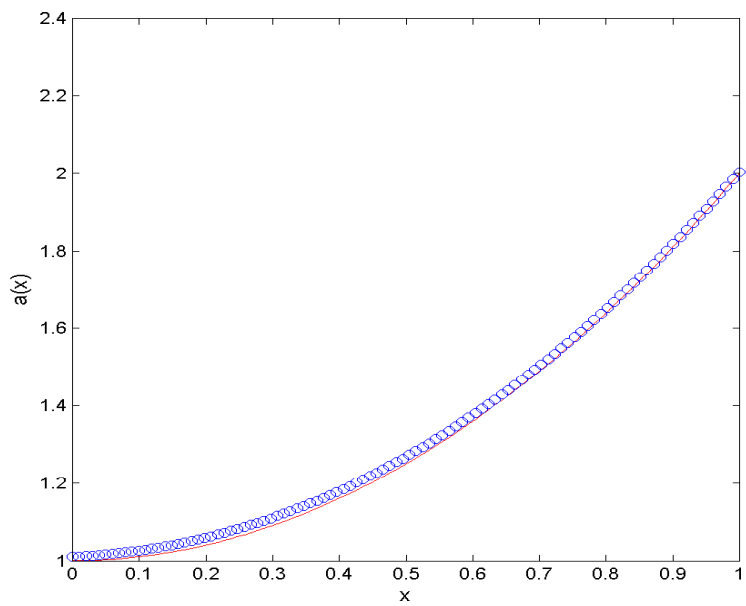


Figure 2.12: Example 4: Inverse Problem

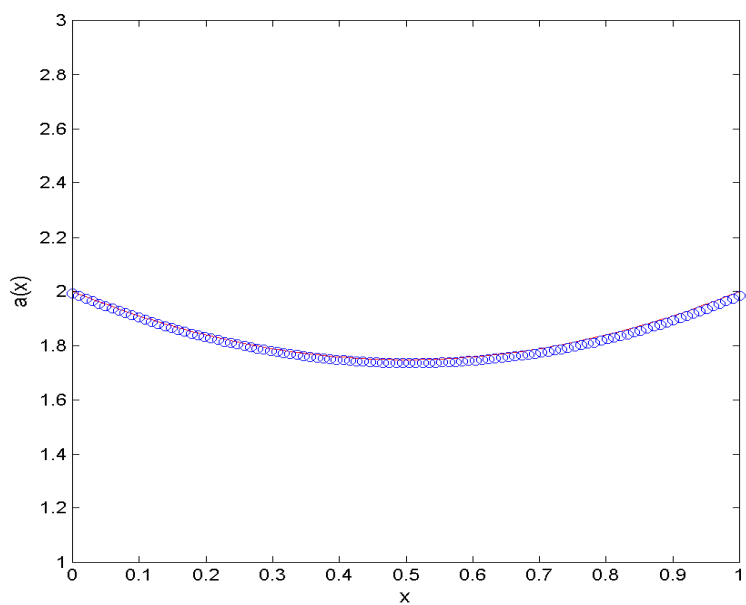


Figure 2.13: Example 5: Inverse Problem

2.6 Equation Error Approach

In this section we utilize the equation error cost functional in the inverse problem algorithm. The equation error approach has two distinct advantages over the OLS approach. Firstly, it leads to a convex optimization problem and hence it only possesses global minimizers. Secondly, the equation approach is computationally inexpensive as there is no underlying variational problem to be solved. On the other hand, a deficiency of the equation error approach is that it relies on differentiating the data and hence it is quite sensitive to the noise in the data.

In the following subsections we will derive the cost functional from the definition of the concepts of equation error. Also, we will show that the minimization problem is uniquely solvable. Then we discretize the cost functional as well as gradient and hessian of the cost functional. Finally, we provide numerical examples of the equation error approach.

2.6.1 Derivation of Cost Functional

The space suitable for the weak formulation is given by

$$V := \{v \in H^2(\Omega) : u = \frac{\partial u}{\partial n} = 0 \text{ on } \Gamma\}. \quad (2.46)$$

The weak formulation of the general fourth-order differential equation is given by: Find $u \in V$ such that

$$\int_{\Omega} a \Delta u \Delta v = \int_{\Omega} f v, \quad \text{for all } v \in V. \quad (2.47)$$

For a fixed pair $(a, w) \in L^\infty(\Omega) \times V$, we define the map $E : V \rightarrow \mathbb{R}$ given by

$$E(a, w)(v) = \int_{\Omega} a \Delta w \Delta v - \int_{\Omega} f v. \quad (2.48)$$

The map $E(a, w)(\cdot)$ is linear and continuous and hence belongs to the topological dual V^* of V . We denote by $e(a, w) \in V$, the image of $E(a, w)$ under the Riesz map, that is

$$\langle e(a, w), v \rangle_V = \int_{\Omega} a \Delta w \Delta v - \int_{\Omega} f v, \quad \text{for all } v \in V. \quad (2.49)$$

Let K be the set of admissible coefficients which we assume to be closed and convex subset of $H^2(\Omega)$. For a fixed $z \in V$, we consider the following regularized minimization problem: Find $a^* \in K$ by solving

$$\min_{a \in K} J(a) = \frac{1}{2} \|e(a, z)\|_V^2 + \frac{\varepsilon}{2} \|a\|_2^2, \quad (2.50)$$

where $\varepsilon > 0$ is a regularizing parameter, $z \in V$ is the data, and $\|\cdot\|_2^2$ is the regularization term.

The following result ensures that the above minimization problem is solvable.

Theorem 2.6.1. *The minimization problem (2.50) is uniquely solvable.*

Proof. The proof is based on standard arguments. Since $J(a) \geq 0$ for every $a \in K$, there exists a minimizing sequence $\{a_n\} \subset K$ such that $\lim_{n \rightarrow \infty} J(a_n) = \inf_{a \in K} J(a)$. From

$$\varepsilon \|a_n\|_2^2 \leq \frac{1}{2} \|e(a_n, z)\|_V^2 + \frac{\varepsilon}{2} \|a_n\|_2^2, \quad (2.51)$$

we deduce that the sequence $\{a_n\}$ is bounded in $\|\cdot\|_2$. Due to the reflexivity of the space $H^2(\Omega)$ and the compact embedding of $H^2(\Omega)$ in $L^\infty(\Omega)$, there exists a subsequence that converges weakly in $H^2(\Omega)$ and strongly in $L^\infty(\Omega)$. Using the same notation for the subsequences as well, we have that $a_n \rightarrow \tilde{a} \in K$ in $L^\infty(\Omega)$. In view of the definition of $e(\cdot, \cdot)$, we have

$$\begin{aligned} \langle e(a_n, z), v \rangle_V &= \int_{\Omega} a_n \Delta z \Delta v - \int_{\Omega} f v, \quad \text{for all } v \in V, \\ \langle e(\tilde{a}, z), v \rangle_V &= \int_{\Omega} \tilde{a} \Delta z \Delta v - \int_{\Omega} f v, \quad \text{for all } v \in V. \end{aligned}$$

By subtracting the above two equations and setting $v = e(a_n, z) - e(\tilde{a}, z)$, we obtain

$$\begin{aligned} \|e(a_n, z) - e(\tilde{a}, z)\|_V^2 &= \int_{\Omega} (a_n - \tilde{a}) \Delta z \Delta (e(a_n, z) - e(\tilde{a}, z)) \\ &\leq \|a_n - \tilde{a}\|_{L^\infty(\Omega)} \|e(a_n, z) - e(\tilde{a}, z)\|_V \|z\|_V. \end{aligned}$$

This ensures that $e(a_n, z) \rightarrow e(\tilde{a}, z)$ in V . By invoking the lower-semicontinuity of the norm $\|\cdot\|_2$, we obtain

$$J(\tilde{a}) = \frac{1}{2} \|e(\tilde{a}, z)\|_V^2 + \frac{\varepsilon}{2} \|\tilde{a}\|_2^2$$

$$\begin{aligned}
 &\leq \lim_{n \rightarrow \infty} \frac{1}{2} \|e(a_n, z)\|_V^2 + \liminf_{n \rightarrow \infty} \frac{\varepsilon}{2} \|a_n\|_2^2 \\
 &= \liminf_{n \rightarrow \infty} \left\{ \frac{1}{2} \|e(a_n, z)\|_V^2 + \frac{\varepsilon}{2} \|a_n\|_2^2 \right\} \\
 &= \inf_{a \in K} J(a).
 \end{aligned}$$

This ensures that $\tilde{a} \in K$ is a solution of (2.50) and the proof is complete. \square

2.6.2 Discretized Cost Functional

The continuous problem (2.50) has to be discretized for a numerical solution. In this work, we will employ finite element discretization on a nondegenerate family $\{\mathcal{T}_h\}$ of triangulations of Ω . We choose A_h to be the finite dimensional space of the coefficient space B . Similarly, V_h will be the finite dimensional subspace of V .

The set K_h of admissible coefficients is given by:

$$K_h = \{v_h \in A_h : \alpha_1 \leq v_h(x) \leq \alpha_2 \ \forall x \in \Omega\}.$$

For any $(a_h, v_h) \in K_h \times V_h$, we define the element $e_h(a_h, v_h) \in V_h$ to be the solution of the variational problem:

$$\langle e_h(a_h, v_h), w_h \rangle_V = \int_{\Omega} a_h \Delta v_h \Delta w_h - \int_{\Omega} f w_h, \quad \text{for all } w_h \in V_h. \quad (2.52)$$

We consider the following discrete minimization problem: Find $a_h \in K_h$ by solving

$$\min_{a \in K_h} J_h(a) = \frac{1}{2} \|e_h(a, z)\|_2^2 + \varepsilon \|a\|_2^2. \quad (2.53)$$

The following result ensures that the continuous problem can be approached by its discrete one.

Theorem 2.6.2. *The discrete minimization problem (2.53) is solvable. If $\{\tilde{a}_h\}_{h>0}$ is a sequence of minimizers of the discrete minimization problem, then each subsequence has a subsequence which converges, in the $L^1(\Omega)$ norm, to a minimizer of the continuous problem (2.50).*

Proof. The existence of minimizers of (2.53) can be proved by using same arguments as employed in the proof of Theorem 2.6.1. Let $\{\tilde{a}_h\}$ be a sequence of minimizers of J_h . Then we have $J_h(\tilde{a}_h) \leq J_h(\alpha_2) \leq C$. Therefore, $\{\tilde{a}_h\}$ remains bounded in BV norm. This further ensures the

existence of a subsequence, still denoted by $\{\tilde{a}_h\}$, which converges to some $\tilde{a} \in K$ in the $L^1(\Omega)$ norm.

Setting $a_h = I_h(\tilde{a}_\tau)$ in (2.53), where $I_h(\cdot)$ is the nodal value interpolant, we have

$$\begin{aligned}
 J(\tilde{a}) &= \frac{1}{2} \|e(\tilde{a}, z)\|_2^2 + \varepsilon \|\tilde{a}\|_2^2 \\
 &\leq \lim_{h \rightarrow 0} \frac{1}{2} \|e_h(\tilde{a}_h, z)\|_2^2 + \liminf_{h \rightarrow 0} \varepsilon \|\tilde{a}_h\|^2 \\
 &\leq \liminf_{h \rightarrow 0} \left\{ \frac{1}{2} \|e_h(\tilde{a}_h, z)\|_2^2 + \varepsilon \|\tilde{a}_h\|_2^2 \right\} \\
 &\leq \liminf_{h \rightarrow 0} \left\{ \frac{1}{2} \|e_h(I_h(\tilde{a}_\tau), z)\|_2^2 + \varepsilon \|I_h(\tilde{a}_\tau)\|_2^2 \right\} \\
 &\leq \frac{1}{2} \|e(\tilde{a}_\tau, z)\|_2^2 + \varepsilon \|a\|_2^2.
 \end{aligned}$$

Since $a \in K$ was chosen arbitrarily, we have shown that $\tilde{a} \in K$ is a minimizer.

□

2.6.3 Cost Functional Gradient Derivation

We recall that for a fixed pair $(a, z) \in K_h \times V_h$, the element $e_h(\cdot, \cdot)$ is defined by

$$\langle e_h(a, z), v \rangle_V = \int_0^1 a z'' v'' - \int_0^1 f v \quad \forall v \in V_h. \quad (2.54)$$

Therefore, for $e_h \in V_h$, we will have $E \in \mathbb{R}^n$, satisfying

$$KE = K(A)Z - F$$

where K is the stiffness matrix defined above coming from the $H^2(\Omega)$ inner product and $Z \in \mathbb{R}^n$ corresponds to the data z . Also, note that K is the stiffness matrix defined previously in 2.2.1. Consequently, we have

$$E(A, Z) = K^{-1}(L(Z)A - F).$$

The above calculation then leads to

$$J(A) = \frac{1}{2} \langle L(Z)A - F, K^{-1}(L(Z)A - F) \rangle_{\mathbb{R}^n}.$$

Let us now compute the gradient and the Hessian of the objective functional. For $\delta A \in \mathbb{R}^m$, we have

$$\begin{aligned} DJ(A)(\delta A) &= \frac{1}{2} \langle L(Z)\delta A, K^{-1}(L(Z)A - F) \rangle_{\mathbb{R}^n} + \frac{1}{2} \langle L(Z)A - F, K^{-1}L(Z)\delta A \rangle_{\mathbb{R}^n} \\ &= \langle \delta A, L(Z)^T K^{-1}(L(Z)A - F) \rangle_{\mathbb{R}^n}, \\ D^2J(A)(\delta A, \delta A) &= \langle L(Z)\delta A, K^{-1}(L(Z)\delta A) \rangle_{\mathbb{R}^n} \\ &= \langle L(Z)^T K^{-1}L(Z)\delta A, \delta A \rangle_{\mathbb{R}^n}. \end{aligned}$$

Summarizing,

$$\begin{aligned} \nabla J(A) &= L(Z)^T K^{-1}(L(Z)A - F) \\ \nabla^2 J(A) &= L(Z)^T K^{-1}L(Z). \end{aligned}$$

2.6.4 Inverse Problem Numerical Examples

In this section we display numerical solutions to the 1-dimensional fourth-order differential equation inverse problem solved on the interval $\Omega = (0, 1)$ with the examples provided in 2.4.3.

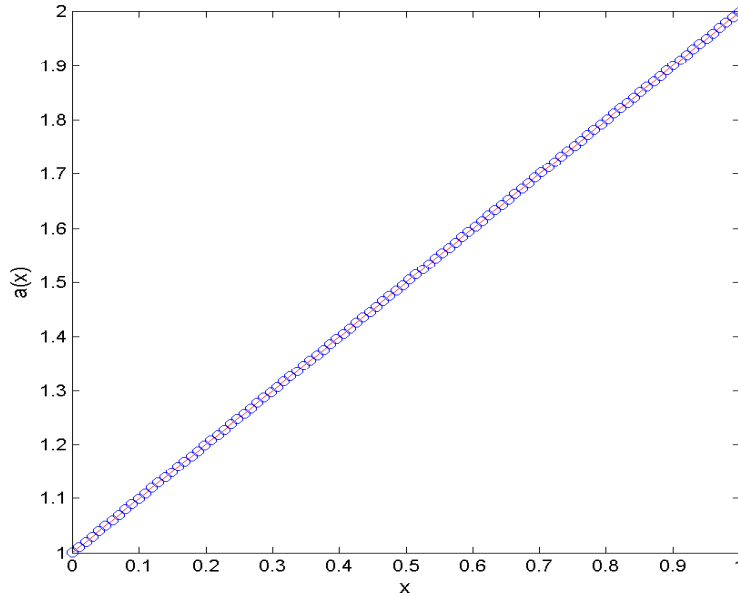


Figure 2.14: Example 1: Inverse Problem

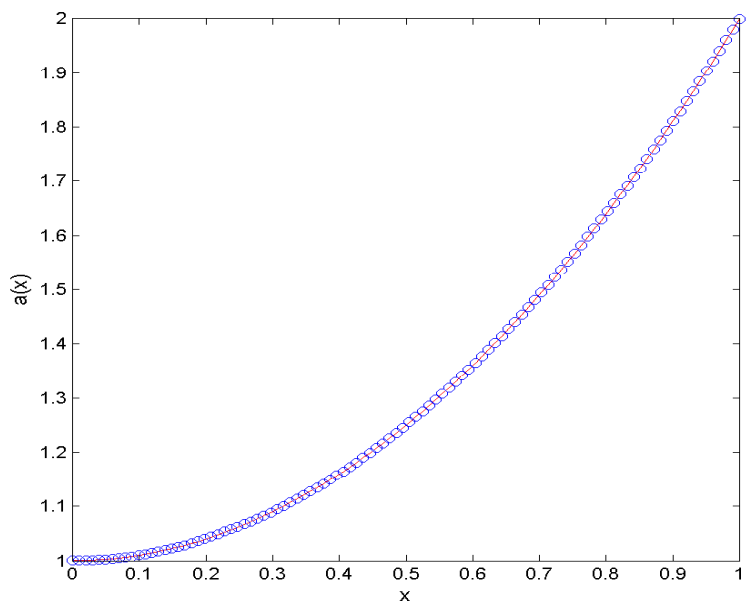


Figure 2.15: Example 2: Inverse Problem

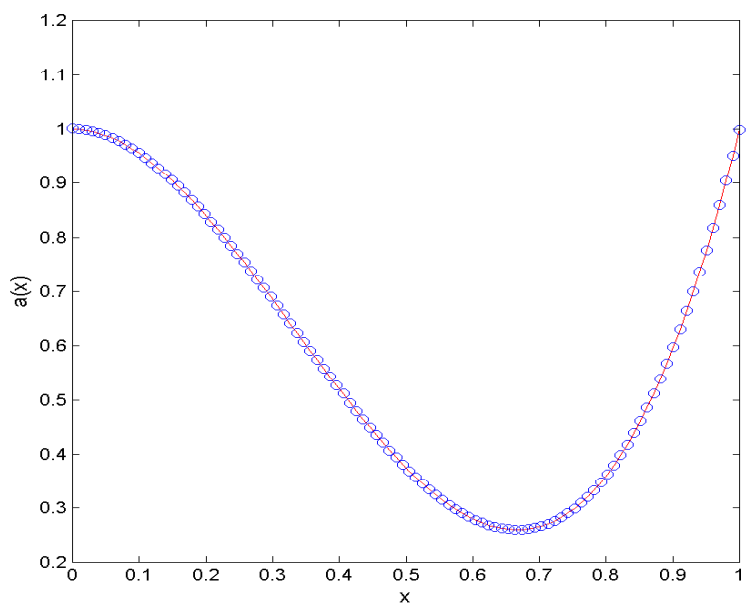


Figure 2.16: Example 3: Inverse Problem

Chapter 3

Parabolic Inverse Problem

In this section we will discuss the inverse problem of identifying a coefficient in a linear parabolic equation. This type of problem is often seen in modeling heat conduction in an isotropic body. Specifically when one wants to identify μ , the heat conductivity of the medium, in the heat equation. The general form of this problem is

$$\gamma \dot{u} - \nabla \cdot (\mu \nabla u) = f \quad \text{in } \Omega \times I,$$

$$u = 0 \text{ on } \Gamma_1 \times I,$$

$$\mu \frac{\partial u}{\partial n} = 0 \text{ on } \Gamma_2 \times I,$$

$$u(x, 0) = u^0(x) \text{ for } x \in \Omega,$$

where $\Omega = \mathcal{R}^d$, $\lambda \in \mathcal{R}$ is heat capacity, $\mu \in \mathcal{R}$ is conductivity, Γ_i is part of the boundary, and $u = u(x, t)$ is the temperature at $x \in \Omega$ and $t \in I = (0, T)$. For more details on this problem we refer to Johnson [5].

We consider a variant of this problem with a spacial variable coefficient and homogeneous Dirichlet boundary conditions. First we will give the general form of the problem and develop the variational form. Then we will discuss the derivation of the Finite Element method solution for solving the direct problem and discuss methods for solving the discrete problem. Finally we will introduce

the related inverse problem of identifying a spacial variable coefficient, discuss the inverse problem methodology, and provide numerical results.

3.1 Direct Problem Formulation

First we establish the general form for the solution of the linear parabolic partial differential equation. For further information on the general parabolic differential equation derivation and alternate methods for solving the problem we refer to several finite element texts [6] [7] [5].

$$\frac{\partial u}{\partial t} - \nabla \cdot (a(x) \nabla u) = f \quad (3.1)$$

$$u = 0 \text{ on } \Gamma \times I, \quad (3.2)$$

$$u(x, 0) = u^0(x) \text{ for } x \in \Omega, \quad (3.3)$$

where $\Omega = \mathcal{R}^d$, Γ is the boundary, $f = f(x, t)$ and $u = u(x, t)$ is the solution of (3.1) at $x \in \Omega$ and $t \in I = (0, T)$. Note that $d = 1, 2$, or 3 correspond to the cases where $x = (x)$, $x = (x, y)$, and $x = (x, y, z)$ respectively.

Next we develop the variational form of the parabolic partial differential equation. We define \mathcal{V} , the linear space of test functions, to be the Hilbert space H_0^1 . By multiplying (3.1) through by $v \in \mathcal{V}$ and applying Green's Formula we obtain the corresponding variational form. The continuous variational problem is to find the solution $u \in \mathcal{V}$ such that

$$\int_{\Omega} \frac{\partial u}{\partial t} v \, dx + \int_{\Omega} a(x) \nabla u \cdot \nabla v \, dx = \int_{\Omega} f v \, dx \quad \forall v \in \mathcal{V} \text{ and } t \in I, \quad (3.4)$$

$$u(x, 0) = u^0(x) \text{ for } x \in \Omega, \quad (3.5)$$

We now introduce \mathcal{V}_h to be the finite dimensional subspace of \mathcal{V} with piecewise linear basis functions over the a discretization of the spacial domain Ω that has step size h . By performing a finite element discretization in space only we create a semi-discretization of the variational form. The discrete variational problem is to find the solution $u_h \in \mathcal{V}_h$ such that

$$\int_{\Omega} \frac{\partial u_h}{\partial t} v \, dx + \int_{\Omega} a(x) \nabla u_h \cdot \nabla v \, dx = \int_{\Omega} f v \, dx \quad \forall v \in \mathcal{V}_h \text{ and } t \in I, \quad (3.6)$$

$$u_h(x, 0) = u^0(x) \text{ for } x \in \Omega, \quad (3.7)$$

Using the definition of the finite dimensional subspace we rewrite $u_h \in \mathcal{V}_h$ as a linear combination of basis functions. We have the following unique representation:

$$u_h(x, t) = \sum_{j=1}^M u_j(t) \phi_j, \quad (3.8)$$

where $u_j(t) \in \mathcal{R}$ are time-dependent coefficients of the basis functions. Next we rewrite (3.6) in terms of basis functions by using (3.8) and letting $v = \phi_i$ for all $i = 1, 2, \dots, n$.

$$\sum_{j=1}^M \frac{\partial u_j(t)}{\partial t} \int_{\Omega} \phi_j \phi_i \, dx + \sum_{j=1}^M u_j(t) \int_{\Omega} a(x) \nabla \phi_j \cdot \nabla \phi_i \, dx = \sum_{j=1}^M \int_{\Omega} f \phi_i \, dx, \quad (3.9)$$

$$\sum_{j=1}^M u_j(0) \phi_j = u_j^0(x) \text{ for } x \in \Omega, i = 1, 2, \dots, n \text{ and } t \in I. \quad (3.10)$$

This fully discretized variational problem as a system of equations suggests the following matrix form.

$$M \frac{d}{dt} U(t) + KU(t) = F \quad (3.11)$$

subject to the initial condition $U(0) = U^0$. The matrices here are defined as

$$M = (m_{ij}) \text{ where } m_{ij} = (\phi_i, \phi_j) = \int_{\Omega} \phi_i \phi_j \, dx, \quad (3.12)$$

$$K = (k_{ij}) \text{ where } k_{ij} = T(a, \phi_i, \phi_j) = \int_{\Omega} a(x) \nabla \phi_i \cdot \nabla \phi_j \, dx, \quad (3.13)$$

$$F_j(t) = (f(t), \phi_j), \quad (3.14)$$

$$U(t) = (u_j). \quad (3.15)$$

Next we explore a method of solving the semi-discrete problem for the u by time discretization. Not all finite difference integration methods are suitable for solving the general parabolic partial differential equation. Implicit methods must be used since the matrix equation of fully discretized

semi-discrete problem (3.11) is generally stiff [5]. Our time discretization of I is to set $0 = t_0 < t_1 < \dots < t_N = T$ and $k_n = t_n - t_{n-1}$ is the local time step. In each method we replace the time derivative with the difference quotient:

$$\frac{d}{dt}u_h(t_n) = \frac{u_h^n - u_h^{n-1}}{k_n} + O(k_n) \quad (3.16)$$

We implement the Backward Euler method. The problem is to find $u_h^n \in \mathcal{V}_h$ for $n = 0, 1, \dots, N$ such that

$$\int_{\Omega} \left(\frac{u_h^n - u_h^{n-1}}{k_n} \right) v \, dx + \int_{\Omega} a(x) \nabla u_h^n \cdot \nabla v \, dx = \int_{\Omega} f(t_n) v \, dx \quad \forall v \in \mathcal{V}_h \text{ and } n = 1, 2, \dots, N, \quad (3.17)$$

$$u(x, 0) = u^0(x) \text{ for } x \in \Omega. \quad (3.18)$$

We represent our solution at each time period as the sum of basis functions.

$$u_h^n = \sum_{j=1}^M u_j^n \phi_j \quad (3.19)$$

Substitution of (3.19) into (3.17) yields the full discretization of the semi-discrete parabolic equation.

$$\sum_{j=1}^M \left(\frac{u_h^n - u_h^{n-1}}{k_n} \right) \int_{\Omega} \phi_j \phi_i \, dx + \sum_{j=1}^M u_j^n \int_{\Omega} a(x) \nabla \phi_j \cdot \nabla \phi_i \, dx = \sum_{j=1}^M \int_{\Omega} f \phi_i \, dx, \quad (3.20)$$

$$\sum_{j=1}^M u_j^0(x, 0) \phi_j = u_j^0(x) \text{ for } x \in \Omega, i = 1, 2, \dots, n \text{ and } t \in I. \quad (3.21)$$

We now rewrite the Backward Euler form of the full discretization in matrix form where we have the notation $U^n = U(t_n)$.

$$M \left(\frac{U^n - U^{n-1}}{k_n} \right) + KU^n = F \quad (3.22)$$

$$U(0) = U^0 \quad (3.23)$$

3.2 FEM Matrix Computations

In this section we derive the discrete finite element matrices that allow us to solve the one-dimensional finite element problem for fourth-order and parabolic partial differential equations. Here we derive the stiffness matrix, denoted K , for the finite element method in one dimension. The stiffness matrix K is defined by the bilinear form $a(\cdot, \cdot)$ from the variational form.

$$K_{ij} = a(\phi_j, \phi_i) \text{ for } i, j = 1, 2, \dots, n \quad (3.24)$$

Note that ϕ_i is zero except on the interval $[x_{i-1}, x_{i+1}]$. Therefore, we see that $a(\phi_j, \phi_i)$ is zero except where the intervals corresponding to ϕ_i and ϕ_j intersect. Thus, $a(\phi_{i-1}, \phi_i)$, $a(\phi_i, \phi_i)$, and $a(\phi_{i+1}, \phi_i)$ are the only nonzero values in K . As a result we have that K is a sparse tri-diagonal matrix.

$$\begin{aligned} K_{j,j} &= \int_{x_{j-1}}^{x_{j+1}} a(x) (\phi'_j)^2 dx \\ &= \frac{1}{h^2} \int_{x_{j-1}}^{x_j} a(x) dx + \frac{1}{h^2} \int_{x_j}^{x_{j+1}} a(x) dx \\ &= \frac{1}{h^2} \cdots \frac{h}{6} \left[a_{j-1} + 4a \left(\frac{x_{j-1} + x_j}{2} \right) + 2a_j + 4a \left(\frac{x_j + x_{j+1}}{2} \right) + a_{j+1} \right] \\ &= \frac{1}{2h} [a_{j-1} + 2a_j + a_{j+1}] \end{aligned} \quad (3.25)$$

from using a simplification that $a\left(\frac{x+y}{2}\right) = \frac{a(x)+a(y)}{2}$.

$$\begin{aligned} K_{j+1,j} &= \int_{x_j}^{x_{j+1}} a(x) \phi'_{j+1} \phi'_j dx \\ &= -\frac{1}{h^2} \int_{x_j}^{x_{j+1}} a(x) dx \\ &= -\frac{1}{6h} \left[a_j + 4a \left(\frac{a_j + a_{j+1}}{2} \right) + a_{j+1} \right] \\ &= -\frac{1}{2h} [a_j + a_{j+1}] \end{aligned} \quad (3.26)$$

Also we note that K is symmetric. So we have that

$$K_{j+1,j} = K_{j,j+1}. \quad (3.27)$$

The load vector F is also derived for the finite element problem in one dimension. The load vector is defined as

$$(f, \phi_i) = \int_{x_{i-1}}^{x_{i+1}} f \phi_i dx = \int_{x_{i-1}}^{x_i} f \phi_i dx + \int_{x_i}^{x_{i+1}} f \phi_i dx \quad (3.28)$$

where (\cdot, \cdot) is the inner product defined on \mathcal{V} .

The integrals evaluated in the computation of the stiffness matrix, mass matrix, and load vector are numerically approximated by Simpson's rule.

$$\int_a^b f(x) dx \approx \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right] \quad (3.29)$$

Below we derive the load vector with piecewise linear basis functions over a one dimensional domain $\Omega = [0, 1]$.

$$\begin{aligned} F_0 &= \int_0^1 \phi_0 f(x) dx \\ &= -\frac{1}{h} \int_{x_0}^{x_1} (x - x_1) f(x) dx \\ &= -\frac{1}{h} \cdot \frac{x_1 - x_0}{6} \left[(x_1 - x_1) f(x_1) + 4 \left(\frac{x_1 + x_0}{2} - x_1 \right) f\left(\frac{x_1 + x_0}{2}\right) + (x_0 - x_1) f(x_0) \right] \\ &= -\frac{1}{h} \cdot \frac{h}{6} \left[4 \left(\frac{x_0 - x_1}{2} \right) \left(\frac{f_1 + f_0}{2} \right) + (-h) f_0 \right] \\ &= -\frac{h}{6} (2f_0 + f_1) \end{aligned} \quad (3.30)$$

where we make the simplifications that $f(x_j) = f_j$ and introduce the approximation that $f\left(\frac{a+b}{2}\right) = \frac{f(a)+f(b)}{2}$. For $j = 1, 2, \dots, n-1$ we have

$$\begin{aligned} F_j &= \int_0^1 \phi_j f(x) dx \\ &= \frac{1}{h} \int_{x_{j-1}}^{x_j} (x - x_{j-1}) f(x) dx - \frac{1}{h} \int_{x_j}^{x_{j+1}} (x - x_{j+1}) f(x) dx \\ &= \frac{1}{h} \cdot \frac{h}{6} \left[(x_j - x_{j-1}) f_{j-1} + 4 \left[\frac{x_j + x_{j-1}}{2} - x_{j-1} \right] f\left(\frac{x_j + x_{j-1}}{2}\right) + (x_j - x_{j-1}) f_j \right] \\ &\quad - \frac{1}{h} \cdot \frac{h}{6} \left[(x_j - x_{j+1}) f_j + 4 \left[\frac{x_j + x_{j+1}}{2} - x_{j+1} \right] f\left(\frac{x_j + x_{j+1}}{2}\right) + (x_{j+1} - x_j) f_{j+1} \right] \end{aligned} \quad (3.31)$$

$$\begin{aligned}
 &= \frac{h}{3} \left[f \left(\frac{x_j + x_{j-1}}{2} \right) + f_j + f \left(\frac{x_j + x_{j+1}}{2} \right) \right] \\
 &= \frac{h}{6} [f_{j-1} + 4f_j + f_{j+1}]
 \end{aligned}$$

$$\begin{aligned}
 F_n &= \int_0^1 \phi_n f(x) dx \\
 &= \frac{1}{h} \int_{x_0}^{x_1} (x - x_{n-1}) f(x) dx \\
 &= \frac{1}{h} \cdot \frac{x_n - x_{n-1}}{6} \left[(x_n - x_{n-1}) f(x_n) + 4 \left(\frac{x_n + x_{n-1}}{2} - x_{n-1} \right) f \left(\frac{x_n + x_{n-1}}{2} \right) \right. \\
 &\quad \left. + (x_{n-1} - x_{n-1}) f(x_{n-1}) \right] \\
 &= \frac{1}{h} \cdot \frac{h}{6} [(-h) f_n] + 4 \left(\frac{x_{n-1} - x_n}{2} \right) \left(\frac{f_n + f_{n-1}}{2} \right) \\
 &= \frac{h}{6} (2f_0 + f_1)
 \end{aligned} \tag{3.32}$$

We compute the mass matrix for the one dimensional problem with piecewise linear basis functions which will be used in following sections.

$$\begin{aligned}
 M_{j,j} &= (\phi_j, \phi_j) \\
 &= \int_{x_{j-1}}^{x_{j+1}} \phi_j^2 dx \\
 &= \frac{1}{h^2} \int_{x_{j-1}}^{x_j} (x - x_{j-1})^2 dx + \frac{1}{h^2} \int_{x_j}^{x_{j+1}} (x - x_{j+1})^2 dx \\
 &= \frac{2}{h^2} \frac{h^3}{3} \\
 &= \frac{2h}{3}
 \end{aligned} \tag{3.33}$$

$$\begin{aligned}
 M_{j,j+1} &= (\phi_j, \phi_{j+1}) \\
 &= \int_{x_j}^{x_{j+1}} \phi_j \phi_{j+1} dx \\
 &= -\frac{1}{h^2} \int_{x_j}^{x_{j+1}} (x - x_{j+1}) (x - x_j) dx \\
 &= -\frac{1}{h^2} \frac{h}{6} [0 + 4(x_{j+1/2} - x_{j+1})(x_{j+1/2} - x_j) + 0] \\
 &= \frac{h}{6}
 \end{aligned} \tag{3.34}$$

$$\begin{aligned}
 M_{j,j+1} &= (\phi_j, \phi_{j+1}) \\
 &= \int_{x_j}^{x_{j+1}} \phi_j \phi_{j+1} dx \\
 &= -\frac{1}{h^2} \int_{x_j}^{x_{j+1}} (x - x_{j+1}) (x - x_j) dx \\
 &= -\frac{1}{h^2} \frac{h}{6} [0 + 4(x_{j+1/2} - x_{j+1})(x_{j+1/2} - x_j) + 0] \\
 &= \frac{h}{6}
 \end{aligned} \tag{3.35}$$

$$M_{j,j-1} = M_{j,j+1} \tag{3.36}$$

3.3 Inverse Problem Formulation

In this section we properly define the inverse problem of identifying a spacial variable coefficient in a parabolic differential equation. We refer to the inverse problem literature for several methods to identify the coefficient [8] [9] [10]. The inverse problem is to identify the coefficient $q(x) \in \mathcal{A}$ that minimizes the Output Least-Squares cost functional $J(q)$. Here \mathcal{A} is the constrained set of admissible coefficients. More specifically it is defined as

$$\mathcal{A} = \{a | a \in \Omega \text{ and } 0 < \alpha_1 \leq q(x) \leq \alpha_2 \text{ where } \alpha_1, \alpha_2 \in \mathcal{R}\} \tag{3.37}$$

The OLS cost functional is

$$J(q) = \frac{k}{2} \int_I \int_{\Omega} |v(q; x, t) - z|^2 dx dt \tag{3.38}$$

where k is the temporal step size, and $v(q; x, t)$ is the solution to the parabolic differential equation associated with a specific coefficient $q \in \mathcal{A}$ and z a finite set of data representing measurements of the solution to the PDE. Minimization of the cost functional converges to the true solution with greater accuracy for convex cost functionals. So, as discussed in previous sections, we add a regularization term to achieve the convexity of the functional. The constrained OLS cost functional with regularization is

$$J(q) = \frac{k}{2} \int_I \int_{\Omega} |v(q; x, t) - z|^2 dx dt + \gamma R(q) \tag{3.39}$$

where γ , the regularization parameter, denotes a positive constant value and

$$R(q) = \int_{\Omega} |\nabla q|^2 dx. \quad (3.40)$$

Now we turn the constrained OLS cost functional into an unconstrained OLS cost functional with the addition of the function $P(q)$ which penalizes the cost functional when q leaves \mathcal{A} .

$$J(q) = \frac{k}{2} \int_I \int_{\Omega} |v(q; x, t) - z|^2 dx dt + \gamma R(q) + \xi \int_{\Omega} P(q) dx \quad (3.41)$$

where ξ is also a small positive constant and $P(\cdot)$ is the projection operator. By discretizing the time domain, $I = (0, T)$, and the spacial domain, Ω , the discrete unconstrained OLS cost functional with regularization is

$$J(q_h) = \frac{k}{2} \sum_{n=1}^M \int_{\Omega} |v_h^n(q_h) - z_h^n|^2 dx + \gamma R(q_h) + \xi \int_{\Omega} P(q_h) dx \quad (3.42)$$

and the discrete projection operator is characterized as

$$P(q_h) = \frac{1}{2} (q_h - \alpha_2)_+^2 + \frac{1}{2} (\alpha_1 - q_h)_+^2. \quad (3.43)$$

Here the notation $(x)_+$ is a function that returns the maximum of x and 0.

Now we derive finite element method of the the adjoint problem. The adjoint problem to the general parabolic partial differential equation was derived to be

$$-\frac{\partial w}{\partial t} - \nabla(a(x)\nabla w) = u - z \quad (3.44)$$

$$w(0, t) = 0 \quad (3.45)$$

$$w(x, T) = 0 \quad (3.46)$$

We find the variational form of the adjoint equation by the standard method. The variational form of the adjoint problem is

$$-\int_{\Omega} \frac{\partial w}{\partial t} v dx + \int_{\Omega} a(x) \nabla w \cdot \nabla v dx = \int_{\Omega} (u - z) v dx \quad \forall v \in \mathcal{V} \quad (3.47)$$

$$w(0, t) = 0 \quad (3.48)$$

$$w(x, T) = 0. \quad (3.49)$$

Introducing a finite difference for the time derivative we obtain the semi-discrete form of the variational adjoint problem.

$$-\int_{\Omega} \frac{(w^n - w^{n-1})}{k_n} v dx + \int_{\Omega} a(x) \nabla w^{n-1} \cdot \nabla v dx = \int_{\Omega} (u^n - z) v dx \quad \forall v \in \mathcal{V} \quad (3.50)$$

$$w^n(0) = 0 \quad \text{for } n = 1, 2, \dots, M \quad (3.51)$$

$$w^M(x) = 0 \quad (3.52)$$

Finally the finite element method of the adjoint problem is: Find w_h^n

$$-\int_{\Omega} \frac{(w_h^n - w_h^{n-1})}{k_n} \phi_h dx + \int_{\Omega} a_h \nabla w_h^{n-1} \cdot \nabla \phi_h dx = \int_{\Omega} (u_h^n - z_h) \phi_h dx \quad \forall \phi_h \in \mathcal{V}_h \quad (3.53)$$

$$w_h^n(0) = 0 \quad \text{for } n = 1, 2, \dots, M \quad (3.54)$$

$$w_h^M(x) = 0 \quad (3.55)$$

Note that the above equation has a terminal condition and must be solved iterating backward through time from $n = M, M-1, \dots, 2, 1$. Now we derive the finite element method matrix form of the variational problem. We represent the solution w_h^n as a linear combination of basis functions.

$$w_h^n = \sum_{j=1}^M w_j^n \phi_j \quad (3.56)$$

Next we use this representation in the previous equation for v_h^n and z as well as for w_h^n .

$$-\sum_{j=1}^M \frac{(w_j^n - w_j^{n-1})}{k_n} \int_{\Omega} \phi_i \phi_j dx + \sum_{j=1}^M w_j^{n-1} \int_{\Omega} a_h \nabla \phi_j \cdot \nabla \phi_i dx = \sum_{j=1}^M \int_{\Omega} (u_j^n - z_j) \phi_j \phi_i dx \quad (3.57)$$

$$w^n(0) = 0 \quad \text{for } n = 1, 2, \dots, M \quad (3.58)$$

$$\sum_{j=1}^M w_j^T(x, T) \phi_j = 0 \quad \text{for } x \in \Omega, i = 1, 2, \dots, n \quad (3.59)$$

The matrix form of the adjoint finite element method is given below:

$$-M \left(\frac{W^n - W^{n-1}}{k_n} \right) + KW^{n-1} = F \quad (3.60)$$

$$W(T) = W^N \quad (3.61)$$

The finite element method of the variational form of the state equation given in (3.62) is

$$\sum_{j=1}^M \left(\frac{u_h^n - u_h^{n-1}}{k_n} \right) \int_{\Omega} \phi_j \phi_i \, dx + \sum_{j=1}^M u_j^n \int_{\Omega} a(x) \nabla \phi_j \cdot \nabla \phi_i \, dx = \sum_{j=1}^M \int_{\Omega} f \phi_i \, dx, \quad (3.62)$$

$$u^n(0) = 0 \text{ for } n = 1, 2, \dots, M \quad (3.63)$$

$$\sum_{j=1}^M u_j^0(x, 0) \phi_j = u_j^0(x) \text{ for } x \in \Omega, i = 1, 2, \dots, n \text{ and } t \in I. \quad (3.64)$$

Equivalently in matrix form, the problem is to find the solution is U to the system of equations:

$$M \left(\frac{U^n - U^{n-1}}{k_n} \right) + KU^n = F \quad (3.65)$$

$$U(0) = U^0 \quad (3.66)$$

We use the above finite element discretizations to solve the state equation and adjoint equation for the approximation of solution u and w respectively. We will use these computations to create a complete discretization of the gradient of the cost functional (3.104) in further sections.

3.4 Derivative Computation

3.4.1 The Fréchet derivative of the parameter to solution operator

The parameter to solution mapping is defined as $F : \mathcal{A} \rightarrow \mathcal{V}$ where the solution belongs to \mathcal{V} , a Hilbert space, and the parameter belongs to \mathcal{A} , a Banach space.

We have that the parameter to solution mapping is given by the general parabolic partial differential equation with homogeneous Dirichlet boundary conditions and a homogeneous initial condition where we view the PDE as a function of the parameter. The strong form is given as

$$\frac{\partial u}{\partial t} - \nabla \cdot (a(x) \nabla u) = f \quad (3.67)$$

$$u = 0 \text{ on } \Gamma \times I, \quad (3.68)$$

$$u(x, 0) = u^0(x) \text{ for } x \in \Omega, \quad (3.69)$$

where $\Omega = \mathcal{R}^d$, Γ is the boundary, $f = f(x, t)$ and $u = u(x, t)$ is the solution of (3.67) at $x \in \Omega$ and $t \in I = (0, T)$.

By application of Green's Formula and applying the boundary conditions we obtain the general variation form of this problem adopting the notation of the trilinear operator.

$$\left(\frac{\partial u}{\partial t}, v \right) + T(a, u, v) = (f, v) \quad \forall v \in \mathcal{V} \quad (3.70)$$

$$u = 0 \text{ on } \Gamma \times I, \quad (3.71)$$

$$u(x, 0) = u^0(x) \text{ for } x \in \Omega, \quad (3.72)$$

where (\cdot, \cdot) denotes the inner product on V and $T(\cdot, \cdot, \cdot)$ is the same trilinear functional as previously defined.

Here we find the Fréchet Derivative of the parameter to solution mapping. We cite the method performed by M. S. Gockenbach and A. A. Khan [4] as an example of this procedure performed in the case of an elliptic partial differential equation. Let $a \in \text{int}(A)$ and δa be a perturbation on a such that $a + \delta a \in A$. Also define $\delta w = F(a + \delta a) - F(a)$ and $u = F(a)$. Note that we can write $F(a + \delta a)$ as $u + \delta w$.

The variational form at a has the form

$$\left(\frac{\partial u}{\partial t}, v \right) + T(a, u, v) = (f, v) \quad \forall v \in \mathcal{V} \quad (3.73)$$

and the variational form at $a + \delta a$ has the form

$$\left(\frac{\partial(u + \delta w)}{\partial t}, v \right) + T(a + \delta a, u + \delta w, v) = (f, v) \quad \forall v \in \mathcal{V} \quad (3.74)$$

Next, we subtract (3.74) from (3.73) and simplify.

$$\begin{aligned} \left(\frac{\partial u}{\partial t}, v \right) + T(a, u, v) - \left(\frac{\partial(u + \delta w)}{\partial t}, v \right) - T(a + \delta a, u + \delta w, v) &= 0 \\ \left(\frac{\partial u}{\partial t}, v \right) + T(a, u, v) - \left(\frac{\partial(u + \delta w)}{\partial t}, v \right) - T(a, u + \delta w, v) - T(\delta a, u, v) - T(\delta a, \delta w, v) &= 0 \\ \left(\frac{\partial(u + \delta w)}{\partial t}, v \right) + T(a, u + \delta w, v) &= \left(\frac{\partial u}{\partial t}, v \right) + T(a, u, v) + T(\delta a, u, v) + T(\delta a, \delta w, v) \end{aligned}$$

This suggests a similar form for the solution for $\delta u = DF(a)\delta a$ where $u = F(a)$ is the parabolic solution. So we have the Fréchet Derivative to the parabolic solution operator is found by solving for δu in

$$\left(\frac{\partial \delta u}{\partial t}, v \right) + T(a, \delta u, v) = -T(\delta a, u, v) \quad \forall v \in \mathcal{V}. \quad (3.75)$$

Equivalently, in less general terms we see that this translates into solving for δu in the equation

$$\int_{\Omega} \frac{\partial \delta u}{\partial t} v dx + \int_{\Omega} a(x) \nabla \delta u \cdot \nabla v dx = - \int_{\Omega} \delta a \nabla u \cdot \nabla v dx \quad \forall v \in \mathcal{V} \quad (3.76)$$

$$u = 0 \text{ on } \Gamma \times I, \quad (3.77)$$

$$u(x, 0) = u^0(x) \text{ for } x \in \Omega, \quad (3.78)$$

3.4.2 Gâteaux Derivative of the Parameter to Solution Operator

Given the weak form of the parabolic differential equation we find the Gâteaux derivative by subtracting the following equations, dividing by ϵ and taking the limit $\epsilon \rightarrow 0$.

$$\left(\frac{\partial u(a)}{\partial t}, v \right) + T(a, u(a), v) = (f, v) \quad \forall v \in \mathcal{V} \quad (3.79)$$

$$\left(\frac{\partial u(a + \epsilon h)}{\partial t}, v \right) + T((a + \epsilon h), u(a + \epsilon h), v) = (f, v) \quad \forall v \in \mathcal{V} \quad (3.80)$$

After subtracting (3.80) from (3.79) we have

$$\left(\left(\frac{\partial u(a)}{\partial t}, v \right) - \frac{\partial u(a + \epsilon h)}{\partial t}, v \right) + T(a, u(a), v) - T((a + \epsilon h), u(a + \epsilon h), v) = 0 \quad \forall v \in \mathcal{V}. \quad (3.81)$$

We collect terms and divide by ϵ .

$$\frac{\left(\frac{\partial u(a+\epsilon h)}{\partial t} - \frac{\partial u(a)}{\partial t}, v\right)}{\epsilon} + \frac{T(a, u(a+\epsilon h) - u(a), v)}{\epsilon} = -T(h, u(a+\epsilon h), v) \quad \forall v \in \mathcal{V} \quad (3.82)$$

Finally, in taking the limit $\epsilon \rightarrow 0$ we have the following expression. If we denote δu to be the derivative of u with respect to h then we have

$$\left(\frac{\partial \delta u(a)}{\partial t}, v\right) + T(a, \delta u(a), v) = -T(\delta h, u(a), v) \quad \forall v \in \mathcal{V}. \quad (3.83)$$

Next we present the general parabolic partial differential equation as a specific example of the above general form.

$$\int_{\Omega} \frac{\partial \delta u}{\partial t} v dx + \int_{\Omega} a(x) \nabla \delta u \cdot \nabla v dx = - \int_{\Omega} h \nabla u \cdot \nabla v dx \quad \forall v \in \mathcal{V} \quad (3.84)$$

$$u = 0 \text{ on } \Gamma \times I, \quad (3.85)$$

$$u(x, 0) = u^0(x) \text{ for } x \in \Omega, \quad (3.86)$$

3.4.3 Deriving the derivative of the OLS cost functional

Before continuing to the derivation of derivative of the cost functional we must define the adjoint equation to the parabolic variational problem (3.70) in order to simplify the computation of the derivative. As defined in the appendix, an adjoint operator A^* of an operator A satisfies the relation that

$$(Ax, y) = (x, A^*y) \quad \forall x, y \in H. \quad (3.87)$$

We seek to find the adjoint differential equation operator of the original parabolic partial differential equation defined in (3.67). It is found by multiplying the operator in (3.67) through by the adjoint variable w , applying Green's Formula, and applying boundary conditions until all partial derivative operators have are passed onto w . The operator defined in equation (3.67) is

$$Au := \frac{\partial u}{\partial t} - \nabla \cdot (a(x) \nabla u) \quad (3.88)$$

Next we derive the adjoint equation.

$$\int_I \int_{\Omega} \left[\frac{\partial u}{\partial t} w - \nabla \cdot (a(x) \nabla w) \right] dx dt \quad (3.89)$$

$$= \int_{\Omega} \left[uw|_0^T - \int_0^T u \frac{\partial w}{\partial t} dt \right] dx - \int_0^T \left[wa(x) \nabla u|_{\Gamma} - \int_{\Omega} a(x) \nabla u \cdot \nabla w dx \right] dt \quad (3.90)$$

$$= \int_{\Omega} \left[uw|_0^T - \int_0^T u \frac{\partial w}{\partial t} dt \right] dx - \int_0^T \left[wa(x) \nabla u|_{\Gamma} + a(x) \nabla w u|_{\Gamma} - \int_{\Omega} \nabla (a(x) \nabla w) u dx \right] dt \quad (3.91)$$

This suggests the boundary conditions for w . The terms evaluated with boundary conditions and initial conditions should evaluate to 0 such that we have

$$\int_0^T \int_{\Omega} -u \frac{\partial w}{\partial t} dx dt - \int_0^T \int_{\Omega} \nabla (a(x) \nabla w) u dx dt. \quad (3.92)$$

where w has the imposed boundary and intial conditions that $w(x, 0) = 0$ and $w = 0$ on Γ . Therefore the adjoint operator is defined by

$$A^* w := -\frac{\partial w}{\partial t} - \nabla \cdot (a(x) \nabla w) \quad (3.93)$$

Finally we achieve the final form of the adjoint equation by imposing the conditions that the operator applied on the domain must equal the state solution u minus the data z . In other words we are essentially setting the right hand side equation to zero.

$$-\frac{\partial w}{\partial t} - \nabla \cdot (a(x) \nabla w) = u - z \quad (3.94)$$

Therefore the weak form, in more general terms, of the adjoint problem is to find the solution $w \in \mathcal{V}$ to the equation

$$-\left(\frac{\partial w}{\partial t}, v \right) + T(a, w, v) = (u - z, v) \quad \forall v \in \mathcal{V} \quad (3.95)$$

$$w = 0 \text{ on } \Gamma \times I, \quad (3.96)$$

$$w(x, T) = u^T(x) \text{ for } x \in \Omega. \quad (3.97)$$

Now that we have the general form of the derivative of the parameter solution mapping we can also calculate the derivative of our cost functional. Consider the OLS cost functional for parabolic partial differential equations defined by

$$J(a) = \int_I (u - z, u - z) \, dt \quad (3.98)$$

Since we wish to minimize the cost functional with respect to a so we take the derivative of $J(a)$ in the direction δa .

$$DJ(a)\delta a = \int_I (\delta u, u - z) \, dt \quad (3.99)$$

Continuing with the derivation of the derivative of (3.98) we use the adjoint equation to simplify (3.99). Note that since the adjoint equation holds for every $v \in V$ then it hold for replacing v with δu . Therefore with this modification we replace the right hand side of (3.95) into (3.99).

$$DJ(a)\delta a = \int_I \left[- \left(\frac{\partial w}{\partial x}, \delta u \right) + T(a, w, \delta u) \right] \, dt \quad (3.100)$$

Next we perform integration by parts on the left most term and apply the initial conditions resulting in

$$DJ(a)\delta a = \int_I \left(w, \frac{\partial \delta u}{\partial x} \right) + T(a, w, \delta u) \, dt \quad (3.101)$$

Another simplification can be made by noticing that the terms inside the time integral are the adjoint equation where u is replaced with δu . The substitution is made.

$$DJ(a)\delta a = \int_I -T(\delta a, u, w) \, dt \quad (3.102)$$

Returning again to the specific case of the general parabolic partial differential equation we have that the derivative of the OLS cost functional is

$$DJ(a)\delta a = - \int_I \int_{\Omega} \delta a \nabla u \cdot \nabla w \, dx \, dt. \quad (3.103)$$

3.4.4 Completing the Gradient Computation

This allows us to complete the computation of the gradient of the cost functional (3.104). We have that the gradient is

$$J'(q_h)p_h = k \sum_{n=1}^M \int_{\Omega} (v_h^n(q_h)'p_h) \cdot (v_h^n(q_h) - z_h^n) \, dx + \gamma R'(q_h)p_h + \xi \int_{\Omega} P'(q_h)p_h \, dx \quad (3.104)$$

where $p_h \in \mathcal{V}_h$ and we see that

$$P'(q_h)p_h = (q_h - \alpha_2)_+ p_h + (\alpha_1)_+ p_h \quad (3.105)$$

and

$$R(q_h)p_h = 2 \int_{\Omega} \nabla q_h \cdot \nabla p_h dx. \quad (3.106)$$

From section 3.4.3 we know that the derivative of the cost functional can be simplified by the computation of the adjoint solution. Therefore the final form of the gradient is

$$J'(q_h)p_h = -k \sum_{n=1}^M \int_{\Omega} p_h \nabla v_h^n(q_h) \cdot \nabla w_h^{n-1} dx + \gamma R'(q_h)p_h + \xi \int_{\Omega} P'(q_h)p_h dx \quad (3.107)$$

3.4.5 Parabolic Cost Function Derivative Computation

In this section we construct the discrete gradient of the cost functional for the general parabolic partial differential equation by finite element method. In the previous section we computed the continuous form of the gradient (3.103). Applying the afore mentioned finite element discretization we derived the discrete gradient as well. Now we give the explicit derivation of the gradient in for the 1D parabolic problem. We first consider the leading term of (3.107) in the following derivation.

From the previous section we have

$$J'(q_h)p_h = -k \sum_{n=1}^M \int_{\Omega} p_h \nabla v_h^n(q_h) \cdot \nabla w_h^{n-1} dx. \quad (3.108)$$

We must use the properties of \mathcal{V}_h to represent $v_h^n(q_h)$ and w_h^{n-1} as a finite sum of basis functions ϕ_i . We represent the state solution and the adjoint solution respectively as

$$v_h^n(q_h) = \sum_{i=1}^N v_i^n \phi_i \quad (3.109)$$

and

$$w_h^{n-1} = \sum_{j=1}^N w_j^{n-1} \phi_j. \quad (3.110)$$

Using these definitions in (3.111), we solve for the components in $J'(q_h)p_h$ corresponding to the l^{th} basis ϕ_l and we obtain

$$g_l = -k \sum_{n=1}^M \sum_{i=1}^N \sum_{j=1}^N \int_{\Omega} \phi_l \nabla (v_i^n \phi_i) \cdot \nabla (w_j^{n-1} \phi_j) dx \quad (3.111)$$

$$= -k \sum_{n=1}^M \sum_{i=1}^N \sum_{j=1}^N \int_{\Omega} \phi_l (v_i^n \phi_i') (w_j^{n-1} \phi_j') dx. \quad (3.112)$$

First we consider the component of ϕ_l corresponding to x_0 .

$$g_0 = -k \sum_{n=1}^M \sum_{i=1}^N \sum_{j=1}^N \int_0^1 \phi_0 (v_i^n \phi_i') (w_j^{n-1} \phi_j') dx \quad (3.113)$$

$$= -k \sum_{n=1}^M \int_{x_0}^{x_1} (\phi_1)^2 v_1^n w_1^{n-1} dx \quad (3.114)$$

$$= -k \sum_{n=1}^M \frac{h}{2} \left(\frac{1}{h^2} \right) v_1^n w_1^{n-1} \quad (3.115)$$

$$= -k \sum_{n=1}^M \frac{1}{2h} v_1^n w_1^{n-1} \quad (3.116)$$

Considering the component of ϕ_l corresponding to x_1 , we see that we have a more complicated intersection of basis functions.

$$\begin{aligned} g_1 &= -k \sum_{n=1}^M \sum_{i=1}^N \sum_{j=1}^N \int_0^1 \phi_1 (v_i^n \phi_i') (w_j^{n-1} \phi_j') dx \\ &= -k \sum_{n=1}^M \left[\int_0^1 \phi_1 (v_1^n \phi_1') (w_1^{n-1} \phi_1') dx + \int_0^1 \phi_1 (v_1^n \phi_1') (w_2^{n-1} \phi_2') dx \right. \\ &\quad \left. + \int_0^1 \phi_1 (v_2^n \phi_2') (w_1^{n-1} \phi_1') dx + \int_0^1 \phi_1 (v_2^n \phi_2') (w_2^{n-1} \phi_2') dx \right] \\ &= -k \sum_{n=1}^M \left[\int_{x_0}^{x_1} \phi_1 (v_1^n \phi_1') (w_1^{n-1} \phi_1') dx + \int_{x_1}^{x_2} \phi_1 (v_1^n \phi_1') (w_1^{n-1} \phi_1') dx \right. \\ &\quad \left. + \int_{x_1}^{x_2} \phi_1 (v_1^n \phi_1') (w_2^{n-1} \phi_2') dx + \int_{x_1}^{x_2} \phi_1 (v_2^n \phi_2') (w_1^{n-1} \phi_1') dx \right. \\ &\quad \left. + \int_{x_1}^{x_2} \phi_1 (v_2^n \phi_2') (w_2^{n-1} \phi_2') dx \right] \\ &= -k \sum_{n=1}^M \left[\left(\frac{h}{2} \right) \left(\frac{1}{h^2} \right) v_1^n w_1^{n-1} + \left(\frac{h}{2} \right) \left(\frac{1}{h^2} \right) v_1^n w_1^{n-1} + \left(\frac{h}{2} \right) \left(\frac{-1}{h^2} \right) v_1^n w_2^{n-1} \right. \\ &\quad \left. + \left(\frac{h}{2} \right) \left(\frac{1}{h^2} \right) v_2^n w_1^{n-1} + \left(\frac{h}{2} \right) \left(\frac{1}{h^2} \right) v_2^n w_2^{n-1} \right] \end{aligned}$$

$$\begin{aligned}
 & + \left(\frac{h}{2} \right) \left(\frac{-1}{h^2} \right) v_2^n w_1^{n-1} + \left(\frac{h}{2} \right) \left(\frac{1}{h^2} \right) v_2^n w_2^{n-1} \Big] \\
 & = -\frac{k}{2h} \sum_{n=1}^M [2v_1^n w_1^{n-1} - v_1^n w_2^{n-1} - v_2^n w_1^{n-1} + v_2^n w_2^{n-1}] \\
 \\
 g_l & = -k \sum_{n=1}^M \sum_{i=1}^N \sum_{j=1}^N \int_0^1 \phi_l (v_i^n \phi'_i) (w_j^{n-1} \phi'_j) dx \\
 & = -k \sum_{n=1}^M \left[\int_0^1 \phi_l (v_{l-1}^n \phi'_{l-1}) (w_{l-1}^{n-1} \phi'_{l-1}) dx + \int_0^1 \phi_l (v_{l-1}^n \phi'_{l-1}) (w_l^{n-1} \phi'_l) dx \right. \\
 & \quad + \int_0^1 \phi_l (v_l^n \phi'_l) (w_{l-1}^{n-1} \phi'_{l-1}) dx + \int_0^1 \phi_l (v_l^n \phi'_l) (w_l^{n-1} \phi'_l) dx \\
 & \quad + \int_0^1 \phi_l (v_l^n \phi'_l) (w_{l+1}^{n-1} \phi'_{l+1}) dx + \int_0^1 \phi_l (v_{l+1}^n \phi'_{l+1}) (w_l^{n-1} \phi'_l) dx \\
 & \quad \left. + \int_0^1 \phi_l (v_{l+1}^n \phi'_{l+1}) (w_{l+1}^{n-1} \phi'_{l+1}) dx \right] \\
 & = -k \sum_{n=1}^M \left[\int_{x_{l-1}}^{x_l} \phi_l (v_{l-1}^n \phi'_{l-1}) (w_{l-1}^{n-1} \phi'_{l-1}) dx + \int_{x_{l-1}}^{x_l} \phi_l (v_{l-1}^n \phi'_{l-1}) (w_l^{n-1} \phi'_l) dx \right. \\
 & \quad + \int_{x_{l-1}}^{x_l} \phi_l (v_l^n \phi'_l) (w_{l-1}^{n-1} \phi'_{l-1}) dx + \int_{x_{l-1}}^{x_l} \phi_l (v_l^n \phi'_l) (w_l^{n-1} \phi'_l) dx \\
 & \quad + \int_{x_l}^{x_{l+1}} \phi_l (v_l^n \phi'_l) (w_l^{n-1} \phi'_l) dx + \int_{x_l}^{x_{l+1}} \phi_l (v_l^n \phi'_l) (w_{l+1}^{n-1} \phi'_{l+1}) dx \\
 & \quad \left. + \int_{x_l}^{x_{l+1}} \phi_l (v_{l+1}^n \phi'_{l+1}) (w_l^{n-1} \phi'_l) dx + \int_{x_l}^{x_{l+1}} \phi_l (v_{l+1}^n \phi'_{l+1}) (w_{l+1}^{n-1} \phi'_{l+1}) dx \right] \\
 & = -k \sum_{n=1}^M \left[\left(\frac{h}{2} \right) \left(\frac{1}{h^2} \right) v_{l-1}^n w_{l-1}^{n-1} + \left(\frac{h}{2} \right) \left(\frac{-1}{h^2} \right) v_{l-1}^n w_l^{n-1} + \left(\frac{h}{2} \right) \left(\frac{-1}{h^2} \right) v_l^n w_{l-1}^{n-1} \right. \\
 & \quad + \left(\frac{h}{2} \right) \left(\frac{1}{h^2} \right) v_l^n w_l^{n-1} + \left(\frac{h}{2} \right) \left(\frac{1}{h^2} \right) v_l^n w_l^{n-1} + \left(\frac{h}{2} \right) \left(\frac{-1}{h^2} \right) v_l^n w_{l+1}^{n-1} \\
 & \quad \left. + \left(\frac{h}{2} \right) \left(\frac{-1}{h^2} \right) v_{l+1}^n w_l^{n-1} + \left(\frac{h}{2} \right) \left(\frac{1}{h^2} \right) v_{l+1}^n w_{l+1}^{n-1} \right] \\
 & = -\frac{k}{2h} \sum_{n=1}^M [v_{l-1}^n w_{l-1}^{n-1} - v_{l-1}^n w_l^{n-1} - v_l^n w_{l-1}^{n-1} + 2v_l^n w_l^{n-1} - v_l^n w_{l+1}^{n-1} - v_{l+1}^n w_l^{n-1} + v_{l+1}^n w_{l+1}^{n-1}] \\
 \\
 g_N & = -k \sum_{n=1}^M \sum_{i=1}^N \sum_{j=1}^N \int_0^1 \phi_N (v_i^n \phi'_i) (w_j^{n-1} \phi'_j) dx
 \end{aligned}$$

$$\begin{aligned}
 &= -k \sum_{n=1}^M \left[\int_0^1 \phi_N (v_N^n \phi'_N) (w_N^{n-1} \phi'_N) dx + \int_0^1 \phi_N (v_N^n \phi'_N) (w_{N-1}^{n-1} \phi'_{N-1}) dx \right. \\
 &\quad \left. + \int_0^1 \phi_N (v_{N-1}^n \phi'_{N-1}) (w_N^{n-1} \phi'_N) dx + \int_0^1 \phi_N (v_{N-1}^n \phi'_{N-1}) (w_{N-1}^{n-1} \phi'_{N-1}) dx \right] \\
 &= -k \sum_{n=1}^M \left[\int_{x_N}^{x_{N+1}} \phi_N (v_N^n \phi'_N) (w_N^{n-1} \phi'_N) dx + \int_{x_{N-1}}^{x_N} \phi_N (v_N^n \phi'_N) (w_N^{n-1} \phi'_N) dx \right. \\
 &\quad \left. + \int_{x_{N-1}}^{x_N} \phi_N (v_N^n \phi'_N) (w_{N-1}^{n-1} \phi'_{N-1}) dx + \int_{x_{N-1}}^{x_N} \phi_N (v_{N-1}^n \phi'_{N-1}) (w_N^{n-1} \phi'_N) dx \right. \\
 &\quad \left. + \int_{x_{N-1}}^{x_N} \phi_N (v_{N-1}^n \phi'_{N-1}) (w_{N-1}^{n-1} \phi'_{N-1}) dx \right] \\
 &= -k \sum_{n=1}^M \left[\left(\frac{h}{2} \right) \left(\frac{1}{h^2} \right) v_N^n w_N^{n-1} + \left(\frac{h}{2} \right) \left(\frac{1}{h^2} \right) v_N^n w_N^{n-1} + \left(\frac{h}{2} \right) \left(\frac{-1}{h^2} \right) v_N^n w_{N-1}^{n-1} \right. \\
 &\quad \left. + \left(\frac{h}{2} \right) \left(\frac{-1}{h^2} \right) v_{N-1}^n w_N^{n-1} + \left(\frac{h}{2} \right) \left(\frac{1}{h^2} \right) v_{N-1}^n w_{N-1}^{n-1} \right] \\
 &= -\frac{k}{2h} \sum_{n=1}^M [2v_N^n w_N^{n-1} - v_N^n w_{N-1}^{n-1} - v_{N-1}^n w_N^{n-1} + v_{N-1}^n w_{N-1}^{n-1}] \\
 \\
 g_{N+1} &= -k \sum_{n=1}^M \sum_{i=1}^N \sum_{j=1}^N \int_0^1 \phi_0 (v_i^n \phi'_i) (w_j^{n-1} \phi'_j) dx \\
 &= -k \sum_{n=1}^M \int_{x_N}^{x_{N+1}} (\phi_N)^2 v_N^n w_N^{n-1} dx \\
 &= -k \sum_{n=1}^M \frac{h}{2} \left(\frac{1}{h^2} \right) v_N^n w_N^{n-1} \\
 &= -k \sum_{n=1}^M \frac{1}{2h} v_N^n w_N^{n-1}
 \end{aligned}$$

3.5 Numerical Examples

3.5.1 Examples of 1-Dimensional Parabolic Direct Problem

In this section we will present numerical solutions to the one-dimensional form of (3.1) on the interval $\Omega = (0, 1)$. We solve the problem

$$\frac{\partial u}{\partial t} - \frac{\partial}{\partial x} \left(a(x) \frac{\partial u}{\partial x} \right) = f \tag{3.117}$$

$$u(0, t) = u(1, t) = 0 \quad (3.118)$$

$$u(x, 0) = u^0(x) \text{ for } x \in \Omega. \quad (3.119)$$

Example 1:

$$u(x, t) = \cos(\pi t) \sin(2\pi x)$$

$$a(x) = 7 - \cos(4\pi x) - 3x$$

$$\begin{aligned} f(x, t) = & -12\pi^2 \cos(\pi t) \sin(2\pi x)x - \pi \sin(\pi t) \sin(2\pi x) - 4\pi^2 \cos(\pi t) \sin(2\pi x)(\cos(4\pi x) - 7) \\ & - 2\pi \cos(\pi t) \cos(2\pi x)(4\pi \sin(4\pi x) - 3 \end{aligned}$$

Example 2:

$$u(x, t) = e^{\sin(\pi t)} \sin(2\pi x)$$

$$a(x) = 6 - x^2 + \sin(2\pi x)$$

$$\begin{aligned} f(x, t) = & (-4\pi^2 e^{\sin(\pi t)} \sin(2\pi x))x^2 + (4\pi e^{\sin(\pi t)} \cos(2\pi x))x - 4\pi^2 e^{\sin(\pi t)} \cos(2\pi x)^2 \\ & + 4\pi^2 e^{\sin(\pi t)} \sin(2\pi x)(\sin(2\pi x) + 6) + \pi e^{\sin(\pi t)} \cos(\pi t) \sin(2\pi x) \end{aligned}$$

Example 3:

$$u(x, t) = 10x^2(x - 1)t^2$$

$$a(x) = 5 + x(x - 1)$$

$$f(x, t) = (20t - 120t^2)x^3 + (150t^2 - 20t)x^2 + (-340t^2)x + 100t^2$$

Example 4:

$$u(x, t) = -x(x - 1/2)(x - 1) \cos(2\pi t)$$

$$a(x) = 5 + 3 \sin(2\pi x)$$

$$\begin{aligned} f(x, t) = & (2\pi \sin(2\pi t))x^3 + (18\pi \cos(2\pi t) \cos(2\pi x) - 3\pi \sin(2\pi t))x^2 + (6 \cos(2\pi t) * (3 \sin(2\pi x) + 5) \\ & + \pi \sin(2\pi t) - 18\pi \cos(2\pi t) \cos(2\pi x))x + 3\pi \cos(2\pi t) \cos(2\pi x) - 3 \cos(2\pi t)(3 \sin(2\pi x) + 5) \end{aligned}$$

The following plots are the parabolic solutions to these examples.

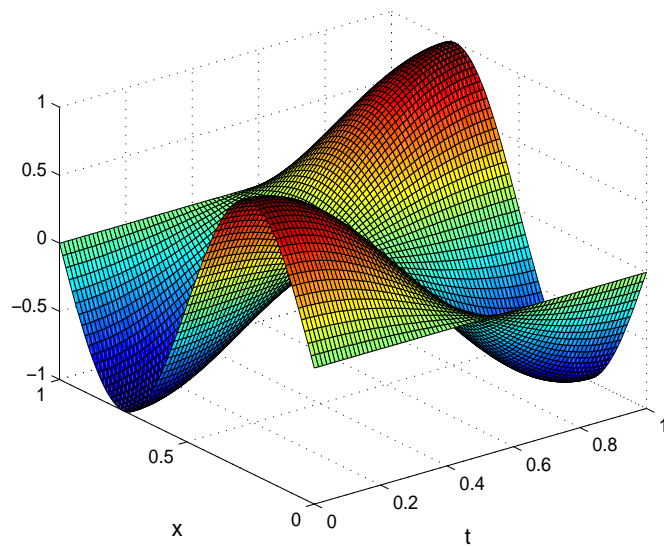


Figure 3.1: Example 1

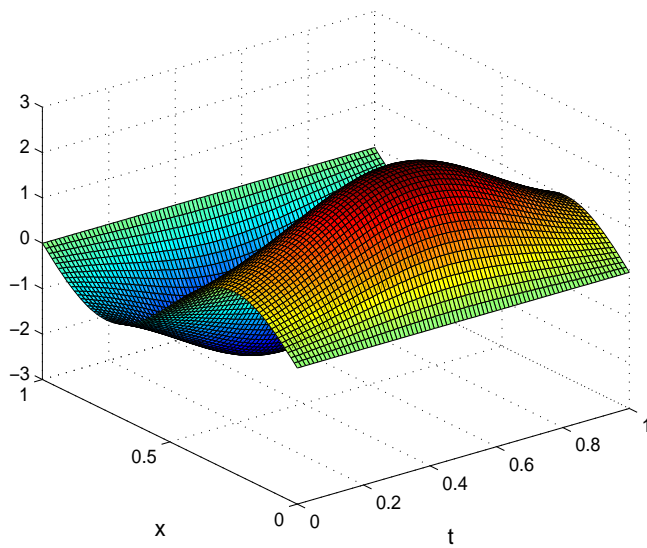


Figure 3.2: Example 2

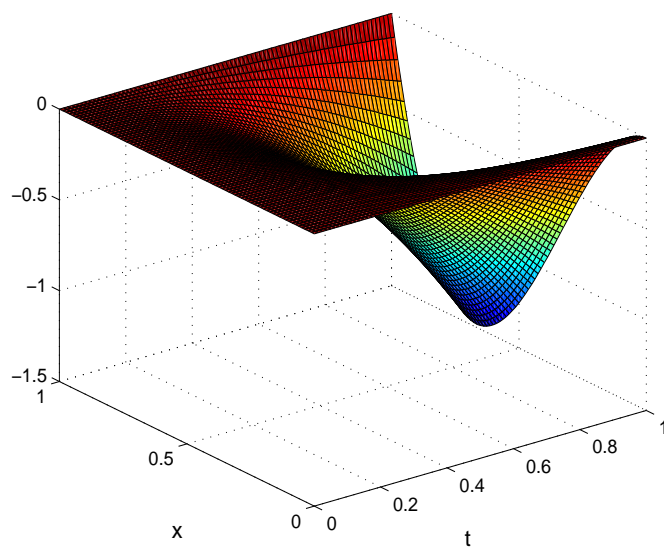


Figure 3.3: Example 3

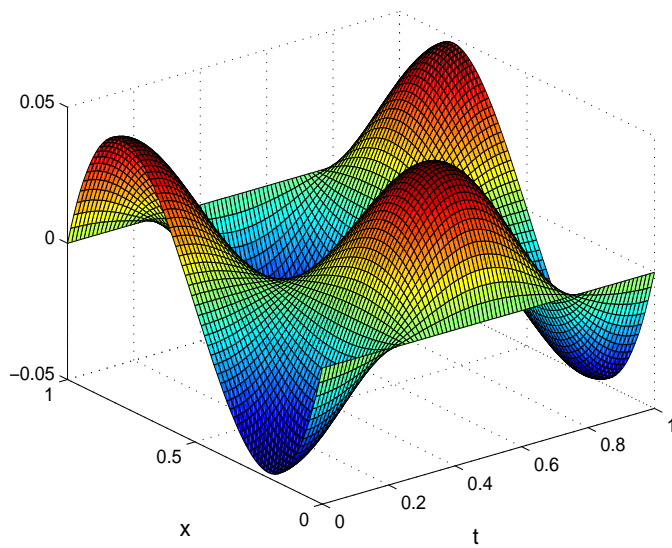


Figure 3.4: Example 4

3.5.2 Examples of 1-Dimensional Parabolic Inverse Problem

The following plots are the recovered coefficients $a(x)$ recovered from the parabolic equations given in 3.5.1 from a discrete measurement of $u(x, t)$ at the terminal observation.

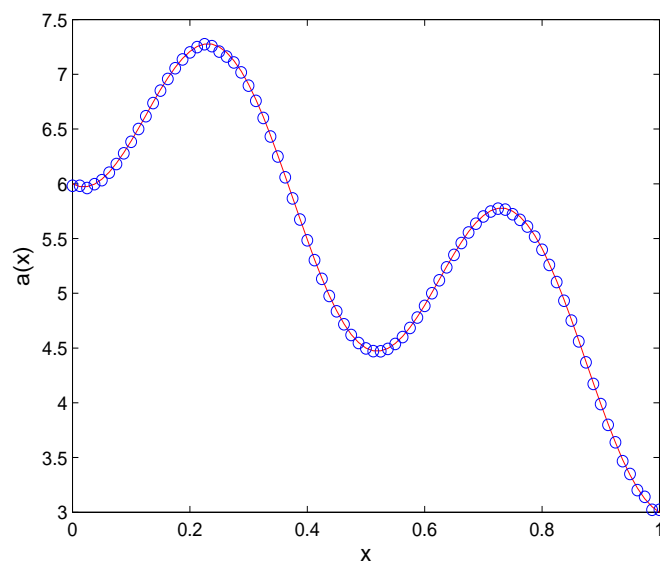


Figure 3.5: Example 1

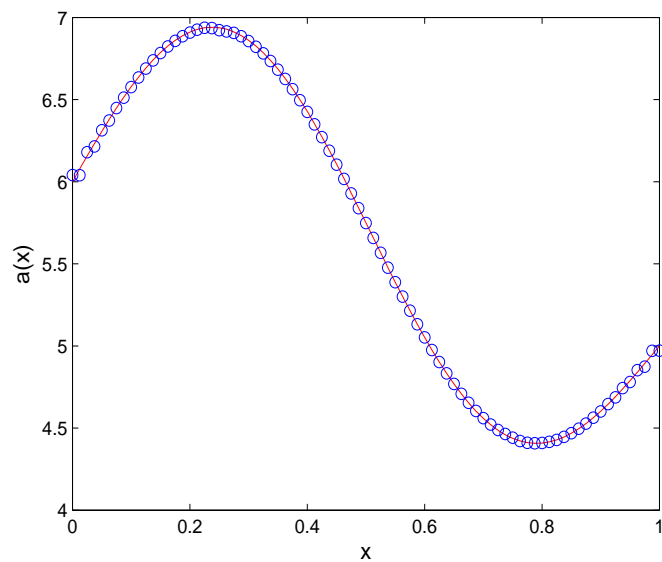


Figure 3.6: Example 2

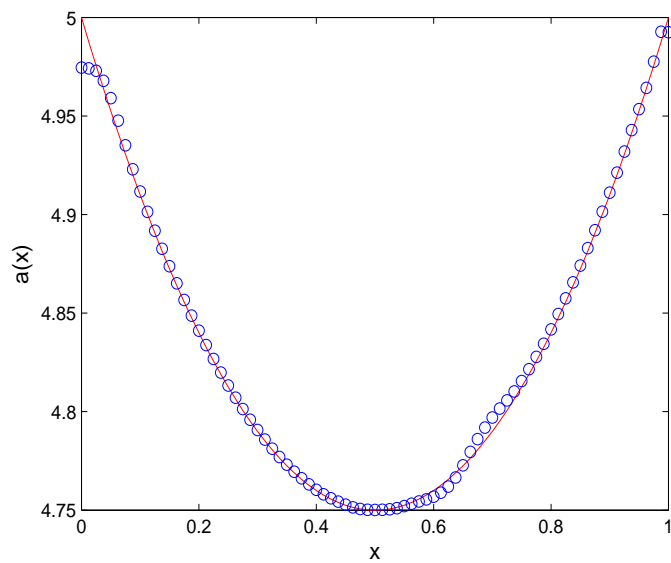


Figure 3.7: Example 3

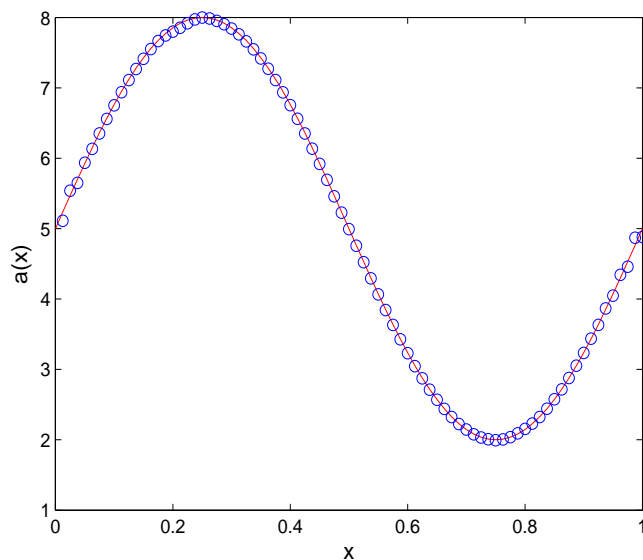


Figure 3.8: Example 4

3.5.3 Examples of 2-Dimensional Parabolic Direct Problem

In this section we display numerical solutions to the 2-dimensional parabolic partial differential equation on the interval $\Omega = (0, 1) \times (0, 1)$. In general form, the problem is to solve

$$\frac{\partial u}{\partial t} - \nabla \cdot (a(x, y) \nabla u) = f \quad (3.120)$$

$$u(x, t) = 0 \text{ on } \Gamma \times I, \quad (3.121)$$

$$u(x, 0) = u^0(x) \text{ for } x \in \Omega. \quad (3.122)$$

Example 1:

$$u(x, y; t) = \cos(\pi t) \sin(2\pi x) \sin(2\pi y)$$

$$a(x, y) = 5 - \cos(4\pi x) \sin(4\pi y)$$

Example 2:

$$u(x, y; t) = 1000x(x - 1)y(y - 1)t^2$$

$$a(x, y) = 5 + 100x(x - 1)y(y - 1)$$

Example 3:

$$u(x, y; t) = \cos(\pi t) \sin(2\pi x) \sin(\pi y)$$

$$a(x, y) = 5 + 10x(x - 1)y$$

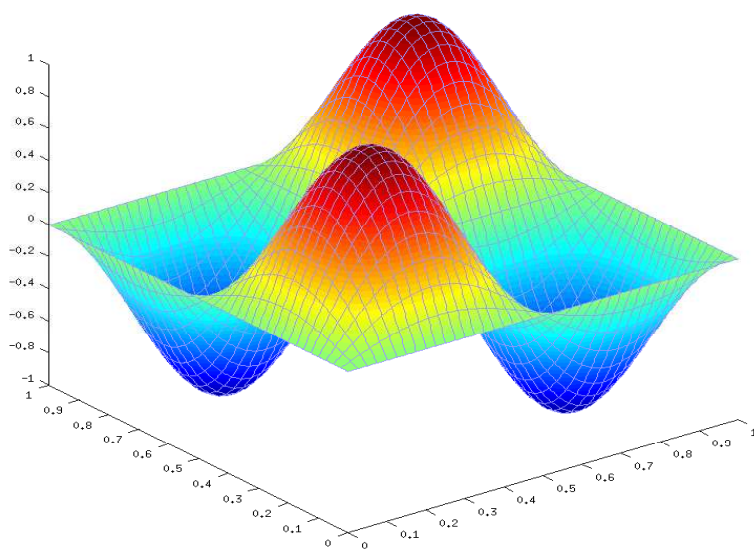


Figure 3.9: Example 1: $t = 0$

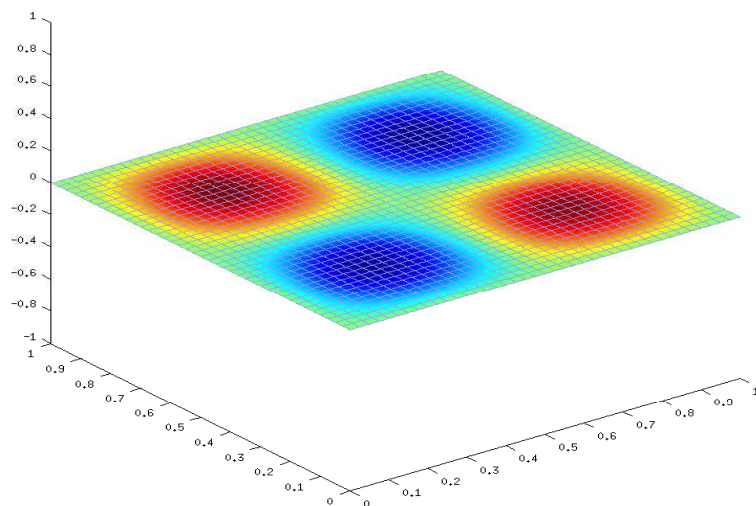


Figure 3.10: Example 1: $t = 0.5$

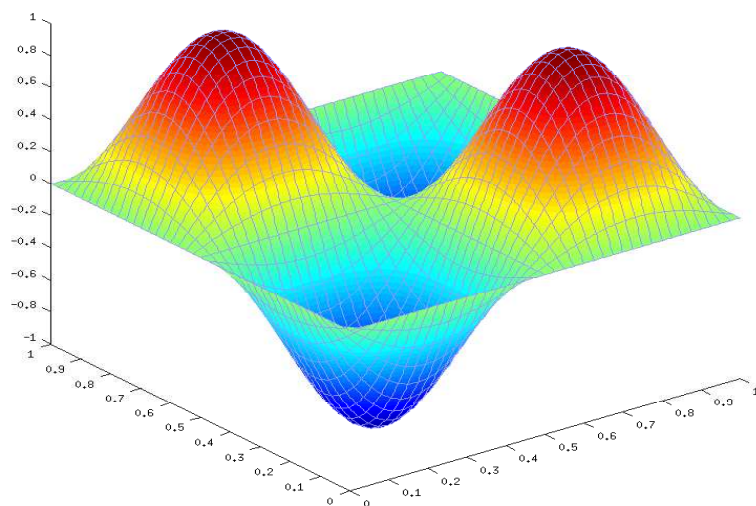


Figure 3.11: Example 1: $t = 1$

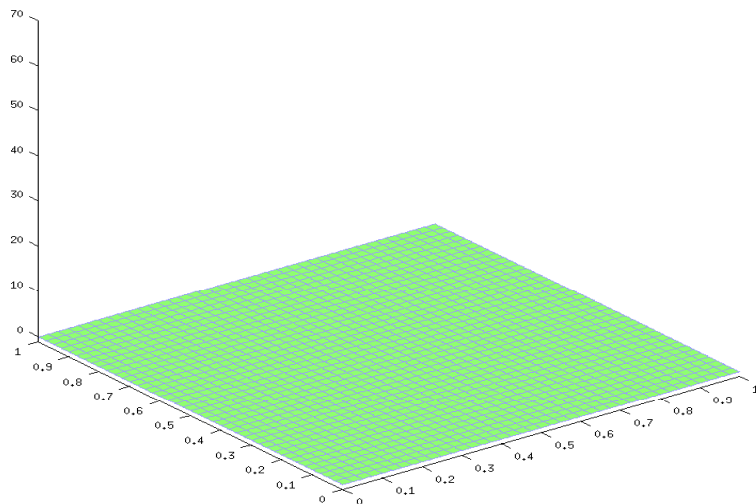


Figure 3.12: Example 2: $t = 0$

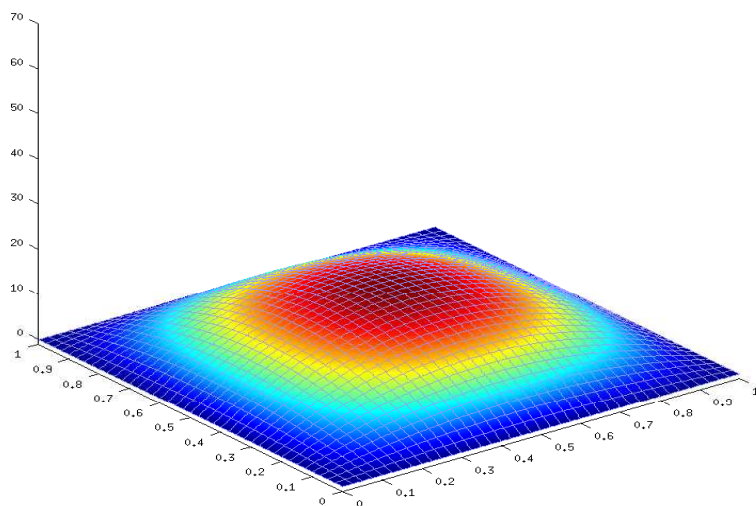


Figure 3.13: Example 2: $t = 0.5$

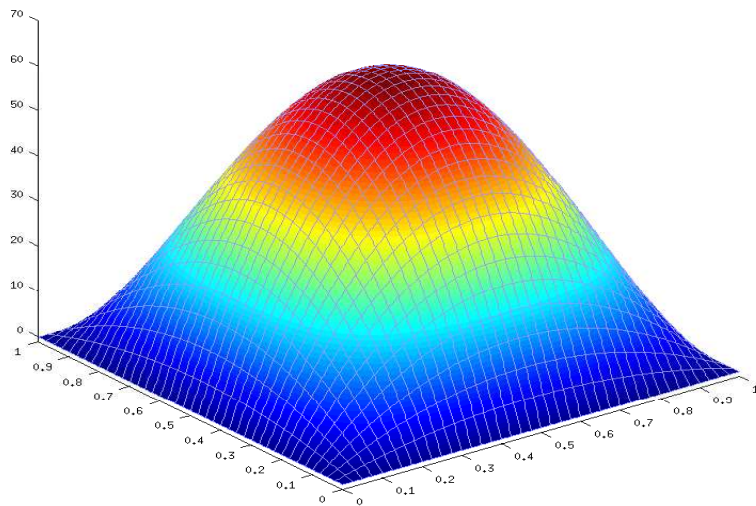


Figure 3.14: Example 2: $t = 1$

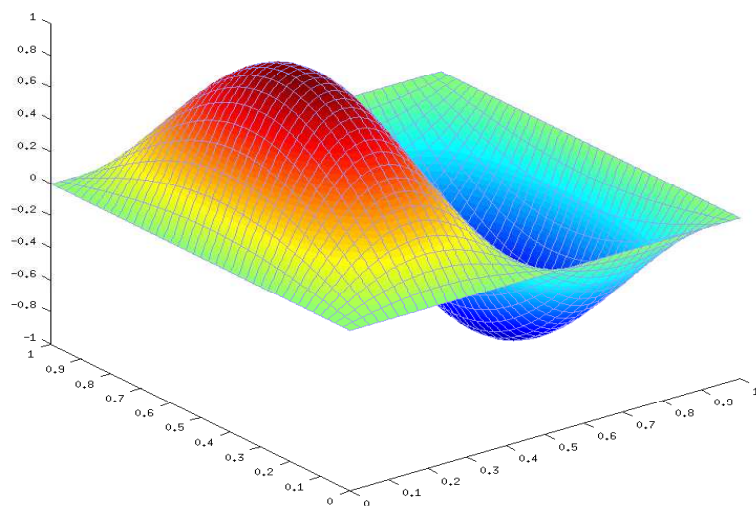


Figure 3.15: Example 3: $t = 0$

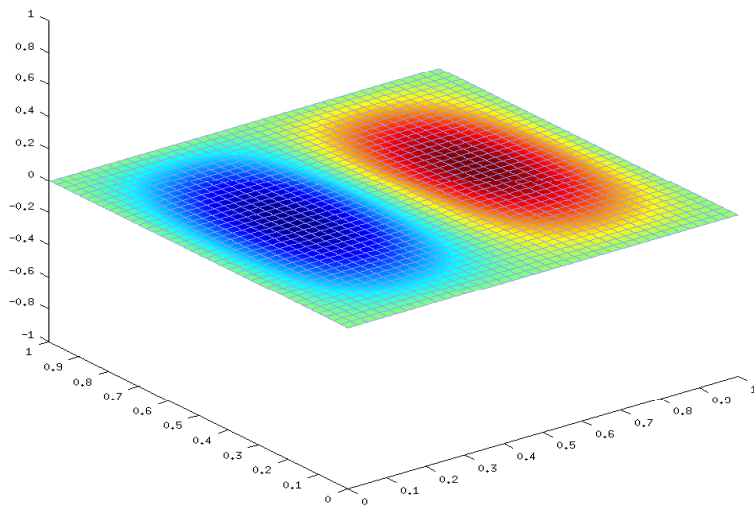


Figure 3.16: Example 3: $t = 0.5$

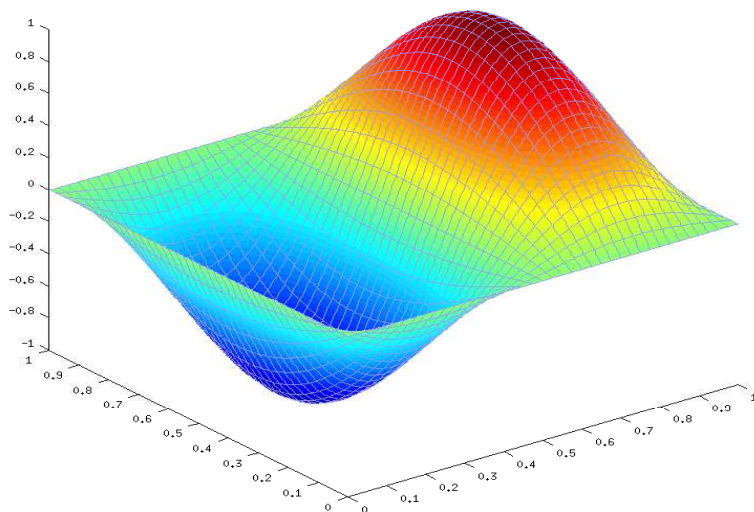


Figure 3.17: Example 3: $t = 1$

3.5.4 Examples of 2-Dimensional Parabolic Inverse Problem

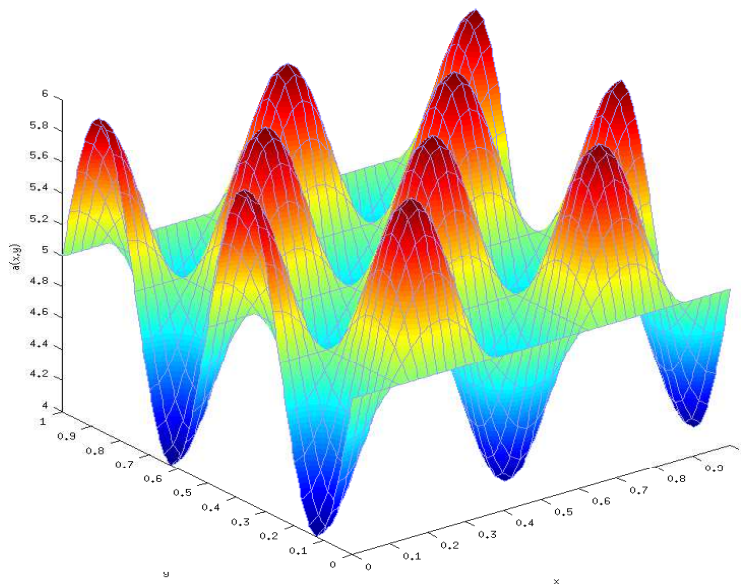


Figure 3.18: Example 1: Exact Coefficient

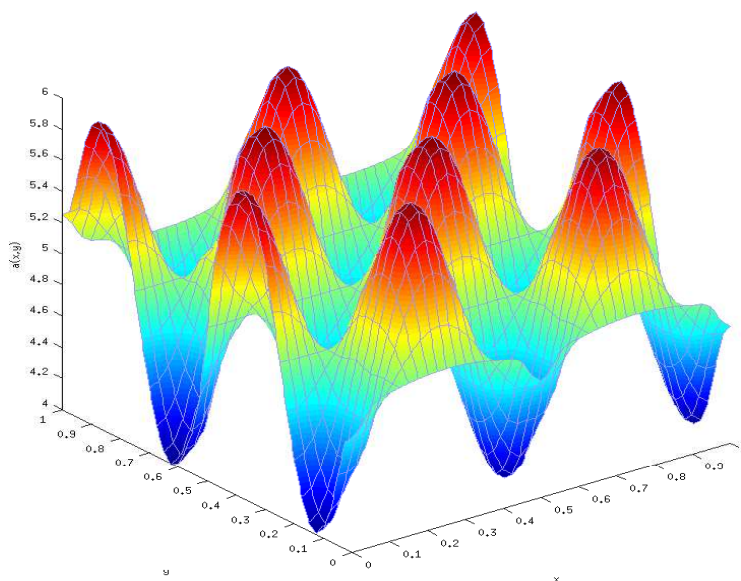


Figure 3.19: Example 1: Estimated Coefficient

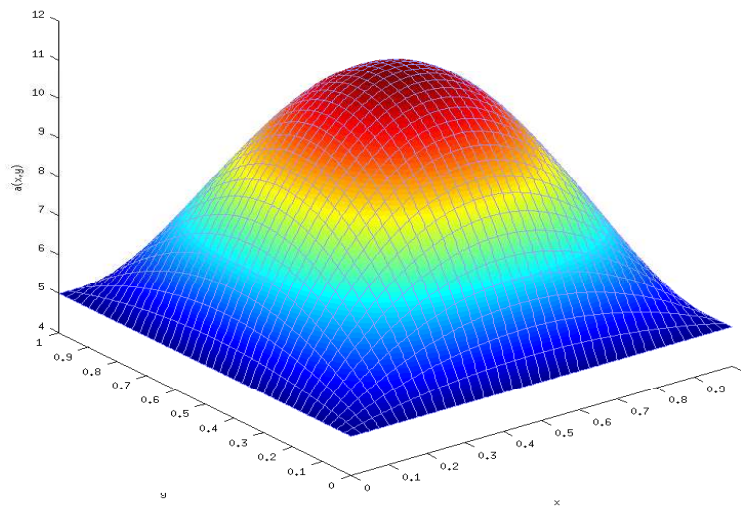


Figure 3.20: Example 2: Exact Coefficient

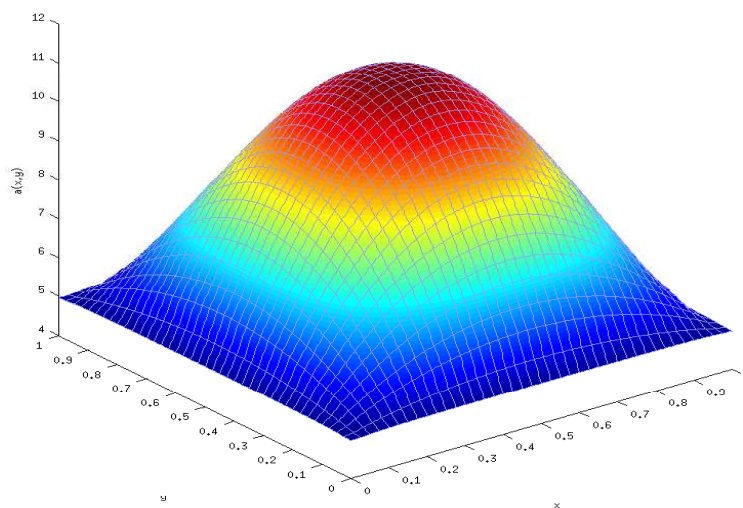


Figure 3.21: Example 2: Estimated Coefficient

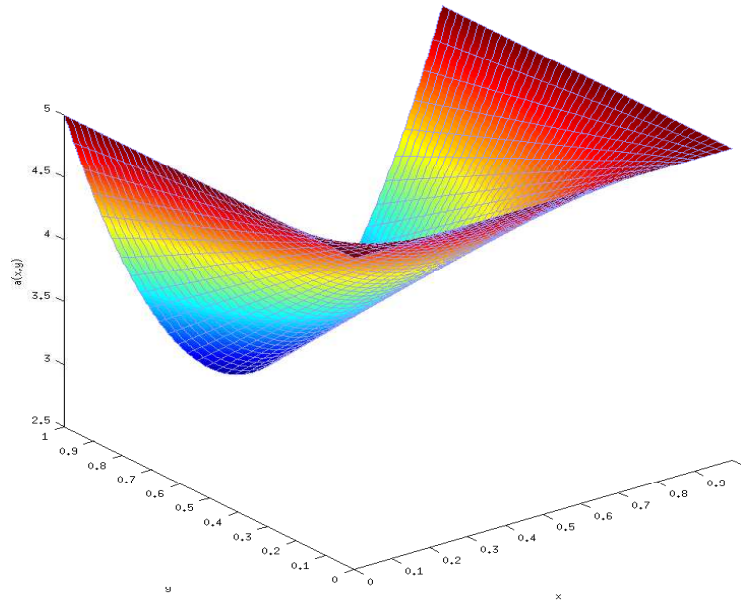


Figure 3.22: Example 3: Exact Coefficient

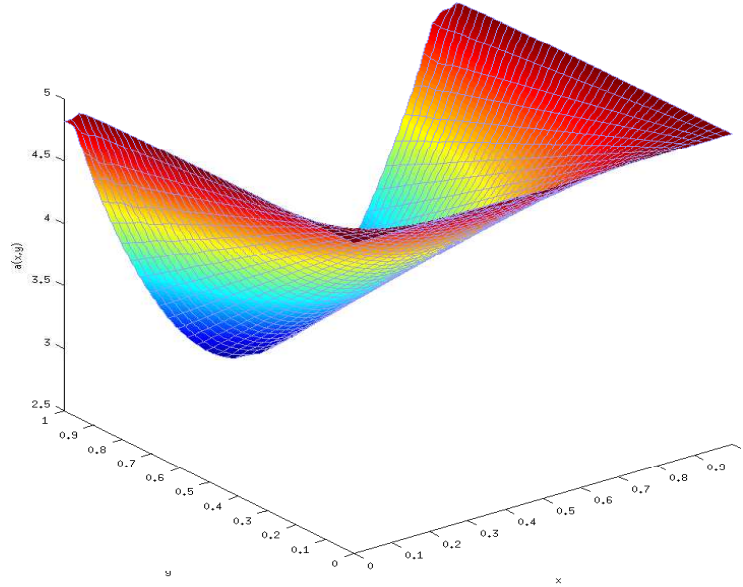


Figure 3.23: Example 3: Estimated Coefficient

Chapter 4

Appendix

4.1 Function Spaces

In the section we compile definitions that are essential for understanding the function spaces implemented throughout the thesis. For more complete definitions we refer to [11].

Definition: (Vector Space). A vector space is a nonempty set X defined over a field K . The vector space has two operations, namely vector addition and multiplication of vectors by elements of K .

Definition: (Normed Space). A normed space is a vector space with a norm defined on it.

Definition: (Complete Space). A space X is said to be complete if every Cauchy sequence in X converges.

Definition: (Banach Space). A normed vector space X is said to be Banach if X is complete.

Definition: (Hilbert Space). A Hilbert space H is a complete vector space with an inner product defined on it (i.e. a complete inner product space).

Definition: (L^1 Space). The space L^1 is the space of integrable functions from Ω to \mathbb{R} with a norm defined as

$$\|f\|_{L^1} = \|f\|_1 = \int_{\Omega} |f| d\mu \quad (4.1)$$

Definition: (L^p Space). Let $p \in \mathbb{R}$ and $1 < p < \infty$, we set

$$L^p(\Omega) = \{f : \Omega \rightarrow \mathbb{R}; f \text{ is measurable and } |f|^p \in L^1(\Omega)\} \quad (4.2)$$

with the norm

$$\|f\|_{L^p} = \|f\|_p = \left[\int_{\Omega} |f(x)|^p d\mu \right]^{1/p} \quad (4.3)$$

Definition: (L^2 space). A specific instance of the above L^p spaces is when $p = 2$ which has special application in the case of Hilbert and Sobolev spaces. This is the space of all square-integrable functions defined by the L^2 -norm.

$$L^2(\Omega) = \{v : \Omega \rightarrow \mathbb{R} : \int_{\Omega} v^2 < \infty\} \quad (4.4)$$

Definition: (H^1 space). The Sobolev space H^1 is defined as

$$H^1(\Omega) = \{v \in L^2(\Omega) : \frac{\partial v}{\partial x_i} \in L^2(\Omega) \text{ for all } i\} \quad (4.5)$$

with the associated norm

$$\|f\|_{H^1} = (\|f\|_{L^2}^2 + \|f'\|_{L^2}^2)^{1/2} \quad (4.6)$$

Definition: (H_0^1 space). The Sobolev space H_0^1 is H^1 with Dirichlet boundary conditions.

$$H_0^1(\Omega) = \{v \in H^1(\Omega) : v = 0 \text{ on } \Gamma\} \quad (4.7)$$

Definition: ($W^{m,p}$ space). Given an integer $m \geq 2$ and a real number $1 \leq p \leq \infty$ we define by

$$W^{m,p}(\Omega) = \{f \in W^{m-1,p}(\Omega); f' \in W^{m-1,p}(\Omega)\}. \quad (4.8)$$

with the notation that $H^m(\Omega) = W^{m,2}(\Omega)$. Is equipped with the norm

$$\|f\|_{W^{m,p}} = \|f\|_{L^p} + \sum_{\alpha=1}^m \|D^{\alpha} f\|_p \quad (4.9)$$

where α is a multi-indices such that $|\alpha| \leq m$.

4.2 The Fréchet Derivative

In this section we are concerned with the differentiability of the parameter to solution mapping. We derive the general form of the Fréchet derivative of the variational problem for elliptic and parabolic partial differential equations.

Definition: Let X and Y be normed vector spaces, and $U \subset X$ be open, and $f : U \rightarrow Y$. Moreover, f is said to be differentiable at $x \in U$ if there exists a bounded linear map $Df(x) \in L(X, Y)^*$ and a continuous function $\phi : V \rightarrow Y$, where V is an open neighborhood of $0 \in X$, with $\phi(0) = 0$, such that

$$f(x + h) = f(x) + (Df(x))h + ||h||\phi(h) \quad (4.10)$$

for all $h \in \mathcal{V}$ and $Df(x)$ is the Fréchet Derivative.

4.3 The Gâteaux Derivative

In this section we similarly calculate the Gâteaux derivative, similar to the Fréchet derivative.

Definition: Let $f : U \subseteq X \rightarrow Y$ where U is open, and X and Y are Banach spaces. The function f is said to be Gâteaux differentiable at $x \in U$ if there exists a bounded linear operator $T : X \rightarrow Y$ such that

$$\lim_{\epsilon \rightarrow 0} \frac{f(x + \epsilon h) - f(x)}{\epsilon} = T_x(h) \quad \forall h \in X \quad (4.11)$$

$\forall h \in X$. Then T is called the Gâteaux derivative of f at x in the direction h .

4.4 Bilinear and Trilinear Form and Properties

The general variational, or weak form, of a boundary value problem must be defined to discuss general finite element existence, uniqueness, convergence, and stability theory.

Find $u \in V$ such that

$$a(u, v) = f(v) \quad \forall v \in \mathcal{V} \quad (4.12)$$

where \mathcal{V} is a Hilbert space and $f \in \mathcal{V}'$, the dual space of \mathcal{V} .

This is called the bilinear form of the boundary value problem while the following form is equivalent and is known as the trilinear form. We have that $a(u, v) = \int_{\Omega} a \nabla u \cdot \nabla v = T(q, u, v)$ for $q \in \mathcal{B}$ where q is the coefficient in the differential equation and \mathcal{B} is the coefficient function space. The difference is that the trilinear form explicitly states the coefficient of the boundary value problem in the abstract representation.

Find $u \in V$ such that

$$T(q, u, v) = f(v) \quad \forall v \in \mathcal{V} \quad (4.13)$$

The variational form contains a function $a : \mathcal{V} \times \mathcal{V} \mapsto \mathbb{R}$ which is a symmetric bilinear function. In other words $a(\cdot, \cdot)$ satisfies the following conditions:

1. $a(u, v) = a(v, u) \quad \forall u, v \in \mathcal{V}$
2. $a(\alpha u + \beta v, w) = \alpha a(u, w) + \beta a(v, w) \quad \forall u, v, w \in \mathcal{V}, \text{ and } \forall \alpha, \beta \in \mathcal{R}$
3. $a(u, u) \geq 0$ and $u = 0$ implies $a(u, u) = 0$.

We also explore two important properties of the symmetric bilinear form that are crucial for the variational form to be effective. The following two properties allow us to define $a(\cdot, \cdot)$ as an inner product on \mathcal{V} which leads to application of the Riesz Representation Theorem. The properties are

Ellipticity: $\exists \alpha > 0$ such that $a(u, u) \geq \alpha \|u\|^2 \quad \forall u \in \mathcal{V}$

Boundedness: $\exists \beta > 0$ such that $a(u, v) \leq \beta \|u\| \|v\| \quad \forall u, v \in \mathcal{V}$.

The Riesz Representation theorem also requires that \mathcal{V} be a Hilbert space. By definition \mathcal{V} is an inner product space defined by the inner product (\cdot, \cdot) . It can also be shown that \mathcal{V} is an inner

product space defined by the inner product $a(\cdot, \cdot)$. We recall the definition of an inner product space.

A vector space, \mathcal{V} , is an inner space defined by the inner product $(\cdot, \cdot) : \mathcal{V}, \mathcal{V} \rightarrow \mathcal{F}$ where \mathcal{F} is a field and (\cdot, \cdot) satisfies the following properties:

1. $(u, v) = (v, u) \forall u, v \in \mathcal{V}$
2. $(\alpha u + \beta v, w) = \alpha(u, w) + \beta(v, w) \forall u, v, w \in \mathcal{V}$, and $\forall \alpha, \beta \in \mathcal{F}$
3. $(u, u) \geq 0$ and $u = 0$ if and only if $(u, u) = 0$.

We see that \mathcal{V} clearly satisfies the properties of a vector space, and to be an inner product we must additionally show that $a(u, u) = 0$ implies $u = 0$. By using the ellipticity of \mathcal{V} we see that $0 \geq \alpha \|u\|^2$ implies $u = 0$. Therefore \mathcal{V} is a inner product space.

Another requirement for \mathcal{V} to be a Hilbert space with respect to $a(\cdot, \cdot)$ is that \mathcal{V} is complete. First we define a norm on \mathcal{V} defined by $a(\cdot, \cdot)$ by $\|v\|_{\mathcal{V}} = \sqrt{a(v, v)}$. Since $a(\cdot, \cdot)$ is elliptic and bounded on \mathcal{V} then we see that

$$\sqrt{\alpha} \|v\| \leq \|v\|_{\mathcal{V}} \leq \sqrt{\beta} \|v\| \quad \forall v \in \mathcal{V}. \quad (4.14)$$

It directly follows from (4.14) that $\|\cdot\|$ and $\|\cdot\|_{\mathcal{V}}$ define equivalent norms so we know that since \mathcal{V} is complete under (\cdot, \cdot) then \mathcal{V} is complete under $a(\cdot, \cdot)$.

Note that it was required that l be a bounded function on \mathcal{V} defined by (\cdot, \cdot) so we must also show that l is bounded on \mathcal{V} defined by $a(\cdot, \cdot)$. We see that

$$\sqrt{\alpha} \|v\| \leq \|v\|_{\mathcal{V}} \implies \|v\| \leq \frac{1}{\sqrt{\alpha}} \|v\|_{\mathcal{V}} \implies |l(v)| \leq \frac{M}{\sqrt{\alpha}} \|v\|_{\mathcal{V}} \quad \forall v \in \mathcal{V}$$

Hence l is bounded and we have the conditions necessary to apply the Riesz representation theorem and other theorems of existence, uniqueness, continuity, and stability to (4.12).

4.5 Existence and Uniqueness Theorems

First we present the Riesz Representation Theorem that shows existence and uniqueness of the solution to (4.12).

Theorem: (the Riesz Representation Theorem) Let \mathcal{V} be a Hilbert space and \mathcal{V}' the dual space of \mathcal{V} . Then we see the following two facts hold:

1. $\forall u \in \mathcal{V}$ the linear functional l defined by $l(v) = (u, v)$ belongs to \mathcal{V}' , and furthermore we see

$$\|l\|_{\mathcal{V}'} = \|u\|_{\mathcal{V}} \quad (4.15)$$

2. $\forall l \in \mathcal{V}' \exists$ a unique $u \in \mathcal{V}$ such that

$$\|l\|_{\mathcal{V}'} = \|u\|_{\mathcal{V}} \text{ and } l(v) = (u, v) \quad \forall v \in \mathcal{V} \quad (4.16)$$

Considering the abstract variational problem to some direct problem we provide more general existence and uniqueness results for the finite element solution than the Riesz Representation Theorem. We omit the proof but it may be found in [6].

Theorem: (the Lax-Milgram lemma) Let \mathcal{V} be a Hilbert space, define the bilinear form $a(\cdot, \cdot) : V \times V \rightarrow R$, and define a linear continuous functional $f(\cdot) : \mathcal{V} \rightarrow \mathcal{R}$. Suppose $a(\cdot, \cdot)$ is bounded and coercive, i.e.,

$$\exists \beta > 0 \text{ s.t. } |a(u, v)| \leq \beta \|u\|_V \|v\|_V \quad \forall u, v \in \mathcal{V}, \text{ and}$$

$$\exists \alpha > 0 \text{ s.t. } |a(v, v)| \geq \alpha \|v\|_V^2 \quad \forall v \in \mathcal{V}.$$

Then, there exists a unique $u \in \mathcal{V}$ to the variational problem (4.12) and we see that the solution u depends continuously on f ;

$$\|u\|_V \leq \frac{1}{\alpha} \|f\|_{V'}.$$

More generally the same result holds true in the case where the solution u and the test function v live in different Hilbert spaces. The following lemma provides this result. Again, we omit the proof

but it may be found in [6].

Theorem: (the Generalized Lax-Milgram lemma) Let \mathcal{W} and \mathcal{V} be Hilbert spaces, define the bilinear form $a(\cdot, \cdot) : \mathcal{W} \times \mathcal{V} \rightarrow \mathcal{R}$, and define a linear continuous functional $f(\cdot) : \mathcal{V} \rightarrow \mathcal{R}$. Suppose the following conditions:

$$\exists \beta > 0 \text{ s.t. } |a(u, v)| \leq \beta \|u\|_{\mathcal{W}} \|v\|_{\mathcal{V}} \quad \forall u \in \mathcal{W} \text{ and } v \in \mathcal{V},$$

$$\exists \alpha > 0 \text{ s.t. } \inf_{u \in \mathcal{W}, \|u\|_{\mathcal{W}}=1} \sup_{v \in \mathcal{V}, \|v\|_{\mathcal{V}} \leq 1} |a(u, v)| \geq \alpha,$$

$$\sup_{u \in \mathcal{W}} |a(u, v)| > 0 \quad \forall 0 \neq v \in \mathcal{V}.$$

Then, there exists a unique $u \in \mathcal{W}$ to the problem: Find $u \in \mathcal{W}$ such that

$$a(u, v) = f(v) \quad \forall v \in \mathcal{V}$$

and furthermore

$$\|u\|_{\mathcal{W}} \leq \frac{1}{\alpha} \|f\|_{\mathcal{V}'}$$

4.6 The Adjoint Operator

We setup the definition of the adjoint by first defining the operator A [12]. Suppose that X is a finite-dimensional inner product space, and A is a linear transformation:

$$A : X \rightarrow X$$

From the Riesz representation theorem we have that there exists a unique $z \in X$ such that

$$(Ax, y) = (x, z) \quad \text{for all } x \in X \tag{4.17}$$

For each $y \in X$ there is an associated $z \in X$ and we have the mapping

$$A^* : X \rightarrow X$$

$$y \rightarrow z$$

or alternatively we can write

$$(Ax, y) = (x, A^*y) \quad \text{for all } x, y \in X$$

Therefore we have the definition of the adjoint operator A^* of the operator A which is derived directly from the Riesz Representation theorem.

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