NUMERICAL APPROACHES ON SHAPE OPTIMIZATION OF ELLIPTIC EIGENVALUE PROBLEMS AND SHAPE STUDY OF HUMAN BRAINS

DISSERATION

Presented in Partial Fulfillment of the Requirements for the Degree Doctor of Philosophy in the Graduate School of the Ohio State University

By
Shu Su, M.A.S.
Graduate Program in Mathematics

The Ohio State University
2010

Dissertation Committee:
Dr. Chiu-Yen Kao, Advisor
Dr. Gregory Baker
Dr. Yuan Lou
ABSTRACT

Shape and topology optimizations have been extensively studied and applied in the conductivity and elasticity settings. Mathematically, these are infinite-dimensional optimization problems and the closed-form solutions for most problems are difficult to find. Thus, numerical approaches are commonly used to solve the problems by using iterative methods.

In the first part of this thesis, a new efficient numerical approach is developed and applied to the elliptic eigenvalue problems which are related to mathematical physics. The study investigates the minimization and maximization of the $k$th eigenvalue and the maximization of the spectrum ratio of the differential operator. Physically, the problem is motivated by the question of determining the optimal vibrating membrane made of two materials with distinct mass densities such that the $k$th frequency or the spectrum ratio of the resulting membrane is extremized. This approach utilizes the Rayleigh’s Principle of eigenvalues and can handle the topology changes automatically. It turns out to be more robust and efficient than the classical level set approach. We further extend the method to solve principle eigenvalue minimization problem on surfaces.

Another topic we studied is related to morphology of human brains. Human brains are highly convoluted surfaces with multiple folds. To characterize the complexity of
these folds and their relationship with neurological and psychiatric conditions, different techniques have been developed to quantify the folding patterns and gyrification of the brain. In the second part of this thesis, a new geometric approach is proposed to measure the gyrification of human brains from magnetic resonance images (MRI). This approach is based on intrinsic 3D measurements that relate the local brain surface area to the corresponding area of a tightly wrapped sheet. Geodesic depth is incorporated into the gyrification computation as well. These quantities are efficiently and accurately computed by solving geometric partial differential equations. The presentation of the geometric framework is complemented with experimental results for brain complexity in typically developing children and adolescents. Using this novel approach, evidence of developmental alterations in brain surface complexity throughout childhood and adolescence is provided.
Dedicated to my family
ACKNOWLEDGMENTS

First and foremost, I would like to thank my advisor Professor Chiu-Yen Kao, for her patience, constant encouragement, and generous support throughout my graduate study at The Ohio State University. I have greatly enjoyed numerous discussions with her and benefited enormously from her advice. Particularly, she always gives me directions with such depth of understanding, breadth of knowledge, and raw intuition for her field of expertise.

I thank Professor Gregory Baker, and Professor Yuan Lou for their time and effort participating in my thesis committee. They have generously given their expertise to improve my work.

I thank the Department of Mathematics for their support. Special thanks go to Cindy Bernlohr for the assistance when I gave birth to my first son.

Lastly, I wish to thank my parents, my husband and kid. This work would be impossible without their love and support.
VITA


2003.7  ......................... B.S. in Mathematics,
                Nanjing University of China.

2010.6  .......................... M.A.S. in Statistics,
                The Ohio State University.

2004-Present ....................... Graduate Teaching Associate,
                The Ohio State University.

PUBLICATIONS

White, T., Su, S., Schmidt, M., Kao, C.-Y., & Sapiro, G., The development of
gyration in childhood and adolescence, Brain & Cognition, 72, 36-45.

FIELDS OF STUDY

Major Field: Mathematics

Specialization: Shape Optimization
# TABLE OF CONTENTS

Abstract ................................................................. ii

Dedication ............................................................. iv

Acknowledgments ....................................................... v

Vita ................................................................. vi

List of Figures .......................................................... x

List of Tables ........................................................... xv

I  Eigenvalue Optimization Problems  1

<table>
<thead>
<tr>
<th>CHAPTER</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>8</td>
</tr>
<tr>
<td>2.1</td>
<td>8</td>
</tr>
<tr>
<td>2.2</td>
<td>9</td>
</tr>
<tr>
<td>2.3</td>
<td>11</td>
</tr>
<tr>
<td>3</td>
<td>18</td>
</tr>
<tr>
<td>3.1</td>
<td>18</td>
</tr>
<tr>
<td>3.1.1</td>
<td>19</td>
</tr>
<tr>
<td>3.1.2</td>
<td>25</td>
</tr>
<tr>
<td>3.2</td>
<td>28</td>
</tr>
<tr>
<td>3.2.1</td>
<td>35</td>
</tr>
<tr>
<td>3.2.2</td>
<td>44</td>
</tr>
</tbody>
</table>

vii
Optimization Problem in $\mathbb{R}^n$ ........................................ 52
  4.1 Numerical Methods ........................................... 52
  4.1.1 Fully Sorting ........................................... 53
  4.1.2 Linear Fractional Programming ................................. 64
  4.1.3 Partial Swapping .......................................... 68
  4.1.4 Gradient at Degenerate Eigenvalues ........................... 71
  4.2 Numerical Results ........................................... 72
  4.2.1 $\max_{\rho} \lambda_k$ ........................................ 73
  4.2.2 Investigating Robin Boundary Parameter $\beta$ ................. 88
  4.2.3 $\max_{\rho} \frac{\lambda_{k+1}}{\lambda_k}$ ............................ 90
  4.3 Discussion and Conclusion ................................... 96

Optimization Problem on Manifolds .................................... 98
  5.1 1D problems ................................................ 99
  5.1.1 Forward Problem ......................................... 99
  5.1.2 Optimization Problem .................................. 105
  5.2 2D problems ............................................... 121
  5.3 Conclusion ................................................ 130

II Gyrification Study .................................................... 132
  6 Introduction .................................................. 133
  7 Materials and Methods ......................................... 138
    7.1 Surface Extraction and Depth Computation ....................... 140
    7.2 Computation of the Corresponding Region on the Outer Hull Surface ........................................... 142
    7.3 Gyrification Indexes ....................................... 144
    7.4 Subjects ................................................ 154
    7.5 Statistical Analyses ..................................... 154
  8 Experimental Results .......................................... 156
    8.1 Demographics ........................................... 156
    8.2 Data Analyses on the Pial Surface ............................ 156
    8.3 Data Analyses on the Outer Hull Surface ....................... 159
8.4 Lateralization of Sulcal Depth and Gyrification Measures 159
8.5 Developmental Differences in Sulcal Depth .............. 162
8.6 Developmental Differences in Gyrification .............. 163
8.7 Comparison with Existing Techniques ................. 163
8.8 Discussion .............................................. 166

9 Conclusion Remarks and Discussion .......................... 170

APPENDICES

A Solutions to the Elliptic Eigenvalue Problems ............. 173

Bibliography .................................................. 186
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>FIGURE</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>An illustration of Krein’s theory in 1D: ([0, L]); the first row shows the minimizers of (\lambda_1) and (\lambda_2), and the second row shows the maximizers of (\lambda_1) and (\lambda_2).</td>
</tr>
<tr>
<td>2.2</td>
<td>An illustration of Cox-McLaughlin’s theory of the minimizer of (\lambda_1).</td>
</tr>
<tr>
<td>3.1</td>
<td>Hat functions in 1D</td>
</tr>
<tr>
<td>3.2</td>
<td>A tent function in 2D</td>
</tr>
<tr>
<td>3.3</td>
<td>5-point stencil for Laplace operator</td>
</tr>
<tr>
<td>3.4</td>
<td>The triangulated mesh with a maximum edge length 0.375.</td>
</tr>
<tr>
<td>3.5</td>
<td>Results of the application of the finite element method to the Dirichlet problem. Left panel shows the first 9 eigenvalues for different mesh sizes, and the right panel plots (\log(\lambda_k^h - \lambda_k)) vs. (\log(h)).</td>
</tr>
<tr>
<td>3.6</td>
<td>Results of the application of the finite difference method to the Dirichlet problem. Left panel shows the first 9 eigenvalues for different mesh sizes, and the right panel plots (\log(\lambda_k^h - \lambda_k)) vs. (\log(h)).</td>
</tr>
<tr>
<td>4.1</td>
<td>Area definition using midpoint rule at a grid point in a rectangular mesh.</td>
</tr>
<tr>
<td>4.2</td>
<td>An example of a uniform triangular mesh with the same area for each triangle.</td>
</tr>
</tbody>
</table>
4.3 An illustration of the partial swapping method. Left panel shows the fully sorting method: switch the density values in the difference sets $A\setminus B$ (light gray region) and $B\setminus A$ (dark gray region). Right panel shows the partial swapping method: switch the density values in the subsets $C$ (light gray region) and $D$ (dark gray region).

4.4 An illustration of the selection of the subsets $C$ and $D$. (cyan regions)

4.5 Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_\rho \lambda_1^D = 18.3951$.

4.6 Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_\rho \lambda_2^D = 42.6309$.

4.7 Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_\rho \lambda_3^D = 47.2711$.

4.8 Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_\rho \lambda_4^D = 70.7599$.

4.9 Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_\rho \lambda_5^D = 9.1975$.

4.10 Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_\rho \lambda_1^N = 18.3951$.

4.11 Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_\rho \lambda_2^N = 29.9931$.

4.12 Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_\rho \lambda_3^N = 2.3839$, $\beta = 1$.

4.13 Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_\rho \lambda_4^R = 31.3343$, $\beta = 10$.

4.14 Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_\rho \lambda_5^R = 24.5825$, $\beta = 1$.

4.15 Investigating Robin parameter $\beta$; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. 

xi
4.16 Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_\rho \lambda_2 / \lambda_1 = 2.5959$. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . ..
5.9 Profiles of density and eigenfunctions at selected iteration steps when calculating $\min \rho \lambda_2$ on manifold $\mathcal{M}$: $\{(x, y)|y = \frac{1}{2}(e^x + e^{-x}), x \in [0, \ln(\pi + \sqrt{\pi^2 + 1})]\}, \ K = \frac{3}{2} \ln(\pi + \sqrt{\pi^2 + 1})$: Changes in eigenvalues $\lambda_{1\text{-}3}$.

5.10 Profiles of density and eigenfunctions at selected iteration steps when calculating $\min \rho \lambda_3$ on manifold $\mathcal{M}$: $\{(x, y)|y = \frac{1}{2}(e^x + e^{-x}), x \in [0, \ln(\pi + \sqrt{\pi^2 + 1})]\}, \ K = \frac{3}{2} \ln(\pi + \sqrt{\pi^2 + 1})$: Changes in eigenvalues $\lambda_{2\text{-}4}$.

5.11 Profiles of density and eigenfunctions at selected iteration steps when calculating $\min \rho \lambda_4$ on manifold $\mathcal{M}$: $\{(x, y)|y = \frac{1}{2}(e^x + e^{-x}), x \in [0, \ln(\pi + \sqrt{\pi^2 + 1})]\}, \ K = \frac{3}{2} \ln(\pi + \sqrt{\pi^2 + 1})$: Changes in eigenvalues $\lambda_{3\text{-}5}$.

5.12 Profiles of density and eigenfunctions at selected iteration steps when calculating $\min \rho \lambda_1$ on manifold $\mathcal{M}$: $\{(x, y)|y = x^{3/2}, x \in [1, 2.431656]\}$, $\ K = 3.647484$: Changes in eigenvalues $\lambda_1$ and $\lambda_2$.

5.13 Profiles of density and eigenfunctions at selected iteration steps when calculating $\min \rho \lambda_2$ on manifold $\mathcal{M}$: $\{(x, y)|y = x^{3/2}, x \in [1, 2.431656]\}$, $\ K = 3.647484$: Changes in eigenvalues $\lambda_{1\text{-}3}$.

5.14 Profiles of density and eigenfunctions at selected iteration steps when calculating $\min \rho \lambda_3$ on manifold $\mathcal{M}$: $\{(x, y)|y = x^{3/2}, x \in [1, 2.431656]\}$, $\ K = 3.647484$: Changes in eigenvalues $\lambda_{2\text{-}4}$.

5.15 Profiles of density and eigenfunctions at selected iteration steps when calculating $\min \rho \lambda_4$ on manifold $\mathcal{M}$: $\{(x, y)|y = x^{3/2}, x \in [1, 2.431656]\}$, $\ K = 3.647484$: Changes in eigenvalues $\lambda_{3\text{-}5}$.

5.16 The eigenfunctions on the manifold $\mathcal{M}$: $z = f(x, y) = \sqrt{1 - x^2 - y^2}$, $x^2 + y^2 \leq 1$. 3D and 2D top views are shown for eigenmodes 1-4.

5.17 Results at selected iteration steps; the region of $\rho_1$ is in cyan, and the region of $\rho_2$ is in magenta. $\min \rho \lambda_1 = 2.6181$.

5.18 Results at selected iteration steps; the region of $\rho_1$ is in cyan, and the region of $\rho_2$ is in magenta. $\min \rho \lambda_2 = 5.7387$. 

xiii
5.19 Results at selected iteration steps; the region of $\rho_1$ is in cyan, and the region of $\rho_2$ is in magenta. $\min_\rho \lambda_3 = 6.2543$. .............................. 128
5.20 Results at selected iteration steps; the region of $\rho_1$ is in cyan, and the region of $\rho_2$ is in magenta. $\min_\rho \lambda_4 = 9.654$. .............................. 129
7.1 Flow chart of the main steps of the proposed GI algorithm. Each figure explains the major steps of the algorithm. .............................. 139
7.2 Axial (1st column), coronal (2nd column), and sagittal (3rd column) slices of the MRI brain volume combined with the pial and outer hull surfaces of one hemisphere (blue lines). The red part on the curve is the intersection of the selected region (frontal lobe here) on the pial surface and the corresponding region on the outer hull surface. Top three slices correspond to Figure 1(d) (pial surface) and bottom three slices correspond to Figure 1(e) (outer hull). .............................. 145
7.3 6 regions of interest on left pial surface (1st column), inflated left pial surface (2nd column), and the left hull surface (3rd column). Frontal lobe is shown in blue, parietal lobe in yellow, temporal lobe in green, medio temporal lobe in cyan, occipital lobe in red, and cingulate cortex in magenta. The region which is not classified is shown in brown. . . 148
7.4 Area definition at a vertex in a triangular mesh. For the vertex at the center (cyan), the area is defined as the total area of the region shown in magenta, which is made up of all the triangles constructed by connecting the vertex (cyan), the centroid (black) of its neighboring triangle and the middle point (yellow) of its neighboring ring in the same triangle. .............................. 152
8.1 Data analyses on the pial surface. Left hemisphere measurements are marked by '+' , and right hemisphere measurements are marked by '*'. 158
8.2 Area ratio of the corresponding region (area on the hull surface for corresponding ROI/hull surface area) for each region on both hemispheres for all subjects. Left hemisphere measurements are marked by '+' , and right hemisphere measurements are marked by '*'. .............................. 160
8.3 Developmental differences between gyrification indexes within different regions for the both hemispheres. .............................. 164
# LIST OF TABLES

<table>
<thead>
<tr>
<th>TABLE</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1</td>
<td>Errors in the eigenvalues determined by the finite element method applied to the Dirichlet problem.</td>
</tr>
<tr>
<td>3.2</td>
<td>Errors in the eigenvalues determined by the finite element method applied to the Neumann problem.</td>
</tr>
<tr>
<td>3.3</td>
<td>Errors in the eigenvalues determined by the finite element method applied to the Robin problem.</td>
</tr>
<tr>
<td>3.4</td>
<td>Errors in the eigenvalues determined by the finite element method applied to the Dirichlet problem with variable coefficient.</td>
</tr>
<tr>
<td>3.5</td>
<td>Errors in the eigenvalues determined by the finite element method applied to the Neumann problem with variable coefficient.</td>
</tr>
<tr>
<td>3.6</td>
<td>Errors in the eigenvalues determined by the finite element method applied to the Robin problem with variable coefficient.</td>
</tr>
<tr>
<td>3.7</td>
<td>Errors in the eigenvalues determined by the finite difference method applied to the Dirichlet problem.</td>
</tr>
<tr>
<td>3.8</td>
<td>Errors in the eigenvalues determined by the finite difference method applied to the Neumann problem.</td>
</tr>
<tr>
<td>3.9</td>
<td>Errors in the eigenvalues determined by the finite difference method applied to the Robin problem.</td>
</tr>
<tr>
<td>3.10</td>
<td>Errors in the eigenvalues determined by the finite difference method applied to the Dirichlet problem with variable coefficient.</td>
</tr>
<tr>
<td>Section</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>-------------</td>
</tr>
<tr>
<td>3.11</td>
<td>Errors in the eigenvalues determined by the finite difference method applied to the Neumann problem with variable coefficient.</td>
</tr>
<tr>
<td>3.12</td>
<td>Errors in the eigenvalues determined by the finite difference method applied to the Robin problem with variable coefficient.</td>
</tr>
<tr>
<td>7.1</td>
<td>Lobe mapping from the labelling of sulcal and gyral regions.</td>
</tr>
<tr>
<td>7.2</td>
<td>Demographic information for the 26 typically developing children between the ages of 8 and 19 years of age.</td>
</tr>
<tr>
<td>8.1</td>
<td>Average area ratio on the pial surface, average area ratio of each corresponding region on the hull surface for each lobe, and the mean value of the normalized average depth.</td>
</tr>
<tr>
<td>8.2</td>
<td>Maximum depth (in mm) for the major sulci by hemisphere and paired t-test showing lateralization.</td>
</tr>
<tr>
<td>8.3</td>
<td>One-way ANOVA test showing developmental differences between localized GI (LGI) for different radius (mm) within different regions.</td>
</tr>
<tr>
<td>8.4</td>
<td>One-way ANOVA test showing differences of localized GI between radius (mm) for each age group in each region.</td>
</tr>
</tbody>
</table>
Part I

Eigenvalue Optimization Problems
CHAPTER 1

INTRODUCTION

Shape and topology optimizations have been of great interest in science and engineering recently. They typically deal with determining the shape of a certain structure such that it is optimal in minimizing a cost function while satisfying given constraints. Most of the time, the objective function is governed by a partial differential equation in certain field.

Shape optimizations have been extensively studied and applied in many different fields. For example, a shape optimization problem in conductivity is proposed to find the shape design of a mixture of two isotropic conductors in a fixed domain that minimizes the weight of a thermal diffuser under a prescribed constraint [1]. A two-phase optimization problem seeks to find the optimal distribution of two elastic components that minimizes the potential energy while satisfying a compliance constraint [59]. A structure design of photonic crystals tries to create periodic structures that exhibit band gaps in their spectrum which is important in the field of optics [32]. An optimization problem in population biology is studied to determine the optimal spatial arrangement of favorable and unfavorable regions for a species to survive [30].

The mathematical formulation of such problems is usually defined as to find a subset in a given domain that minimizes an objective function subject to a compliance
constraint. In many cases, the objective functions depend on the solutions of partial differential equations which model the related phenomena. These are infinite-dimensional optimization problems and the closed-form solutions for most problems are difficult to find. Thus, numerical approaches are commonly used to solve the problems by using iterative methods. The classical method for shape optimizations is based on the shape derivative [45, 57] which measures the sensitivity of boundary variation. It is a very popular approach which can handle any type of objective functions and structure models, but this method suffers from two main drawbacks: It requires a smooth parametrization of the boundary and it is difficult to accommodate topological changes. Another method which has been under study is the homogenization method [1, 7]. It is developed to relax smoothness and topological constraints inherent in the classical method. However, it is mainly limited to linear elasticity and particular objective functions. The level set method introduced by Osher and Sethian [47] has been widely applied recently. This numerical technique makes it very easy for performing numerical computations involving curves and surfaces. By representing a shape implicitly as a level set function, which is positive inside the shape, zero on the boundary of the shape, and negative outside of the shape, one can evolve this function instead of the shape boundary itself. This approach is well known for its ability to handle topological changes. Nonetheless, the level set method can get trapped in a local optimum with fewer holes than the global one in some applications. To overcome this disadvantage, modified level set methods [9] incorporating the shape derivatives have been proposed.

In this work, focus is placed on the study of structural vibration control of acoustic
drum problems. Given a vibrating system, we are interested in controlling its resonant frequencies by changing the geometry of the structure under certain constraints. Physically, this problem is motivated by the question of determining the optimal distribution of two materials (different densities) with prescribed mass constraint so that the $k$th frequency of the resulting membrane is extremized. In mathematical terms, consider a drumhead with a fixed bounded domain $\Omega \in \mathbb{R}^n$ and a variable density $\rho(x)$. The resonant frequencies are the solutions to the eigenvalue problem

\[-\Delta u = \lambda \rho u, \quad x \in \Omega,\]
\[u = 0, \quad x \in \partial \Omega.\]  

(1.1)

Assume the density function $\rho(x)$ is a piecewise function which takes on two values

\[\rho(x) = \begin{cases} 
\rho_1, & \text{if } x \in D, \\
\rho_2, & \text{if } x \notin D,
\end{cases}\]  

(1.2)

where $D \subset \Omega$ is an unknown subset of $\Omega$. This originates from reduction of the wave equation. Spectral theory shows that there is an unbounded discrete set of positive eigenvalues

\[0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots\]  

(1.3)

where each $\lambda_k$ is counted with its multiplicity. We want to find an optimal configuration of the density function that solves the following optimization problems

\[
\min_{\rho(x)} \lambda_k \quad \text{or} \quad \max_{\rho(x)} \lambda_k \quad \text{or} \quad \max_{\rho(x)} \lambda_{k+1}/\lambda_k,\]  

(1.4)

subject to the mass constraint

\[\int_{\Omega} \rho dx = K,\]  

(1.5)
where $K$ is a prescribed constant. Imposing different boundary conditions, such as the Neumann boundary and the Robin type boundary conditions to the above optimization problems are also investigated. Depending on the boundary conditions, the optimal density distributions are different. The main objective of this research is to develop an advanced algorithm which satisfies the binary constraint on the density function and can handle the topological changes more efficiently.

Theoretical results of the one-dimensional (1D) case where the class of fixed endpoint strings was considered have been investigated by M. G. Krein [34]. The minimum or maximum $k$th eigenvalue was characterized explicitly using the nodal domains of eigenfunctions. Motivated by Krein’s arguments in 1D, Cox and McLaughlin [13] developed in high dimension a geometric characterization of the extremizers of the first eigenvalue in terms of the level sets of the corresponding eigenfunctions. The numerical simulation in finding a two-phase drum with the deepest bass note based on their theoretical work was performed by Cox [11]. Osher and Santosa [48] then solved the above optimization problem by using the level set method and the projected gradient method [53]. The Lagrange multiplier method was adopted to deal with the constraint. At each iteration, the gradient descent direction was computed and if this direction took the current level set function out of the feasible set, a projection approach was used to put the iterate back onto the feasible set. Using this method, they were able to address the optimization problems of $\min_\rho \lambda_1$, $\min_\rho \lambda_2$, and separation of the spectral gap $\max_\rho (\lambda_2 - \lambda_1)$. However, due to the limitations of getting stuck at local optimum by the classical level set method, the modified level set method including the topological derivatives [2, 3, 9, 19, 22] has become a standard
tool for solving most shape optimization problems. Recently, the variants under the framework of the piecewise constant level set method (PCLSM) become attractive and have been very successful in practice [37, 38, 39, 61]. PCLSM can use one level set function to distinguish multiphase regions and thus can create holes during the evolution of the level set function without topological derivatives. Thus, more complicated shapes can be generated than the classical level set method. Another type of method in maximizing band gap between two consecutive eigenvalues is based on semidefinite programming (SDP) and subspace methods [44]. It turns out to be efficient and robust in handling the optimal design of photonic band structure problems. A survey of some optimal configurations regarding symmetry and symmetry-breaking properties is presented in [10, 49].

Previous work has mainly focused on the Dirichlet boundary conditions, the extremization of the first eigenvalue, and on simple domains. In this work, I develop algorithms for solving more generalized problems, e.g., general boundary conditions, such as the Neumann boundary and Robin type boundary conditions, general eigenvalues as stated in (1.4) and even in the domain of manifolds. I build upon previous work [28] and propose a new iterative approach for the optimization of elliptic eigenvalue problems.

Part I of the thesis is organized as follows. In Chapter 2, the main tools used to study the elliptic eigenvalue problems and basic results of the theory will be reviewed. In Chapter 3, I investigate how to solve the eigenvalues and eigenfunctions of the elliptic eigenvalue equation when $\rho(x)$ is given. The finite element method and the finite difference method will be discussed in detail. In Chapter 4, I propose a new
approach based on the variational form of the eigenvalues and the theoretic work on the gradient at a degenerate eigenvalue by Cox [12]. The proposed methods are applied to problems with different boundary conditions and the numerical results for extremizing eigenvalues and maximizing the spectral ratios are illustrated. In Chapter 5, I solve the shape optimization problems on manifolds. Most of the results are solved on a half unit circle and a half unit sphere even though the method generally works for any surface given as the graph of a function. Future studies are needed for more complicated manifolds.
CHAPTER 2
PRELIMINARIES

In this chapter I review the main tools used to study elliptic eigenvalue equations: Sobolev spaces, variational formulations and basic results of the theory. For further details, the reader is referred to textbooks on partial differential equations (PDEs), e.g., [16] and [17].

2.1 Sobolev Spaces

Let $\Omega$ be a bounded open set in $\mathbb{R}^n$ and $\Gamma$ be its boundary. Denote by $L^2(\Omega)$ the Hilbert space of square integrable functions defined on $\Omega$. The Sobolev space of order 1 is defined by:

$$H^1(\Omega) := \left\{ w \in L^2(\Omega) : \frac{\partial w}{\partial x_i} \in L^2(\Omega), \ i = 1, 2, \ldots n \right\}. \quad (2.1)$$

This is a Hilbert space with respect to the scalar product

$$(w, v)_1 := \int_\Omega w(x)v(x)dx + \int_\Omega \nabla w(x) \cdot \nabla v(x)dx, \quad (2.2)$$

with norm

$$||w||_1 := \left( \int_\Omega \int_\Omega |w(x)|^2dx + \int_\Omega |\nabla w(x)|^2dx \right)^{1/2}. \quad (2.3)$$
The subspace

$$H_0^1(\Omega) := \{ w \in H^1(\Omega) : w|_\Gamma = 0 \}$$  \hspace{1cm} (2.4)$$

is the closure of $C^\infty$ functions compactly supported in $\Omega$ for the norm $|| \cdot ||_1$. From the Poincare inequality

$$\exists C = C(\Omega) \text{ such that } \forall w \in H_0^1(\Omega), \int_\Omega w(x)^2 dx \leq C \left( \int_\Omega |\nabla w|^2 dx \right),$$  \hspace{1cm} (2.5)$$

where $C$ is a constant, depending only on $\Omega$.

Sobolev spaces with a negative exponent can be defined by duality. We use

$$H^{-1}(\Omega) = \text{dual of } H_0^1(\Omega) := \sup \{ f, w \mid w \in H_0^1(\Omega), ||w||_{H_0^1(\Omega)} = 1 \}. \hspace{1cm} (2.6)$$

2.2 Elliptic Eigenvalue Problem

The aim is to study eigenvalue optimization problem for composite membranes. Physically, this problem is motivated by the question of determining the optimal distribution of the two materials (different densities) with prescribed mass constraint so that the $k^{th}$ frequency of the resulting membrane is extremized. In mathematical terms, consider the following eigenvalue optimization problem:

$$-\Delta u_k = \lambda_k(\rho(x)) u_k \quad \text{in} \quad \Omega,$$

$$u_k = 0 \quad \text{on} \quad \partial \Omega,$$

where $\Omega$ is a bounded domain in $\mathbb{R}^n$ with smooth boundary $\partial \Omega$, the density function $\rho(x)$ is non-negative and defined on the admissible set

$$\mathcal{A} := \left\{ \rho \in L^\infty(\Omega) : \alpha \leq \rho(x) \leq \beta \text{ a.e. in } \Omega, \int_\Omega \rho(x) = c \right\} \hspace{1cm} (2.7)$$
with $0 \leq \alpha < \beta$, and $\alpha|\Omega| < c < \beta|\Omega|$. The minimizers or maximizers of a given eigenvalue $\lambda_k(\rho)$ among all $\rho \in \mathcal{A}$ are considered here.

**Rayleigh’s Principle.** The Rayleigh quotient of the Laplace operator is defined as:

$$R_\rho[w] = \frac{\int_{\Omega} |\nabla w|^2 \, dx}{\int_{\Omega} \rho w^2 \, dx}.$$  \hfill (2.9)

Then,

$$\lambda_k(\rho) = \min_{w \in H^1_0(\Omega)} R_\rho[w],$$

$$w \text{ orthogonal to } u_1, u_2, \ldots, u_{k-1}$$

where $u_1, u_2, \ldots, u_{k-1}$ are the first $(k-1)$th eigenfunctions. The minimum is achieved at the corresponding eigenfunction.

**Min-max Principle.** An alternative expression for $\lambda_k(\rho)$, which does not require knowledge of $u_{k-1}$ to obtain $u_k$ is the min-max formula:

$$\lambda_k(\rho) = \min_{E_k \in H^1_0(\Omega)} \max_{w \in E_k, w \neq 0} R_\rho[w],$$

subspace of dim $k$

where the minimum is achieved when $E_k$ is the space spanned by the first $k$th eigenfunctions.
2.3 Main Results

The basic properties of the eigenvalues $\lambda_k$ and the eigenfunctions $u_k$, restated here, are available in [23].

**Theorem 2.3.1.** The map $\rho \to \lambda_k(\rho)$ is continuous on $A$ for the weak-* convergence. Moreover, the map $\rho \to 1/\lambda_k(\rho)$ is convex.

**Theorem 2.3.2. (general existence result)** Let $F : \mathbb{R}^k \to \mathbb{R}$ be a continuous function. Then the problem

$$
\min_{\rho \in A} F(\lambda_1(\rho), \lambda_2(\rho), \cdots, \lambda_k(\rho))
$$

(2.12)

where $A$ is defined in (2.8) has a solution. The same result holds for a similar maximization problem.

**Theorem 2.3.3.** There exists a function $\rho^*$ minimizing $\lambda_k(\rho)$ in the class $A$ defined in (2.8) and it is of the form $\rho^* = \beta \chi_D + \alpha \chi_{\Omega \setminus D}$ for some subset $D$ of $\Omega$.

**Theorem 2.3.4. (Friedland)** Let $F : \mathbb{R}^k \to \mathbb{R}$ be a continuous function, increasing with respect to its arguments. Then the problem

$$
\min_{\rho \in A} F(\lambda_1(\rho), \lambda_2(\rho), \cdots, \lambda_k(\rho))
$$

(2.13)

where $A$ is defined in (2.8) has a solution $\rho^*$ which is of the kind

$$
\rho^* = \beta \chi_D + \alpha \chi_{\Omega \setminus D}
$$

(2.14)
where $D$ is some subset of $\Omega$.

The same result holds for a maximization problem with a function $F$ decreasing with respect to its arguments.

More precise results for the one-dimensional case are derived by M.G. Krein [34], and presented next.

**Theorem 2.3.5. (Krein)**

(i) The (unique) minimizer of $\lambda_1(\rho)$ in the class $A$ defined in (2.8) is the function $\rho_1(x)$ defined by

$$
\rho_1(x) = \begin{cases} 
\alpha & x \in (0, \frac{L}{2} - \delta), \\
\beta & x \in \left(\frac{L}{2} - \delta, \frac{L}{2} + \delta\right), \\
\alpha & x \in \left(\frac{L}{2} + \delta, L\right),
\end{cases}
$$

where $\delta = (c - \alpha L)/2(\beta - \alpha)$.

(ii) The (unique) minimizer of $\lambda_k(\rho)$ in the class $A$ is the function $\rho_k(x)$ which is $L/k$–periodic and which is defined on each interval

$$
(jL/k, (j + 1)L/k), \ j = 0, \cdots, k - 1
$$

by

$$
\rho_k(x) = \rho_1(kx - jL).
$$

(See the first row in Figure 2.1 for the minimizers of $\lambda_1$ and $\lambda_2$.)
Theorem 2.3.6. (Krein)

(i) The (unique) maximizer of $\lambda_1(\rho)$ in the class $\mathcal{A}$ defined in (2.8) is the function $\rho^1(x)$ defined by

$$\rho^1(x) = \begin{cases} 
\beta & x \in (0, \frac{L}{2} - \delta), \\
\alpha & x \in (\frac{L}{2} - \delta, \frac{L}{2} + \delta), \\
\beta & x \in (\frac{L}{2} + \delta, L),
\end{cases}$$

(2.18)

where $\delta = (\beta L - c)/2(\beta - \alpha)$.

(ii) If $\alpha > 0$, the (unique) maximizer of $\lambda_k(\rho)$ in the class $\mathcal{A}$ is the function $\rho^k(x)$ which is $L/k$-periodic and defined on each interval $(jL/k, (j + 1)L/k)$, $j = 0, \ldots, k - 1$ by

$$\rho^k(x) = \rho^1(kx - jL).$$

(2.19)

(See the second row in Figure 2.1 for the maximizers of $\lambda_1$ and $\lambda_2$.)

(iii) If $\alpha = 0$, the maximizers of $\lambda_k(\rho)$ in the class $\mathcal{A}$ are all the functions defined in the following way. Let $\delta_0 = c/2\beta$ and $0 = x_0 < x_1 < x_2 < \cdots < x_{k-1} < x_k = L$ be any sequence of points satisfying the conditions $x_i - x_{i-1} \geq 2\delta_0/k$ ($i = 1, 2, \cdots, k$). Then, the maximizers are the functions $\rho$ defined by

$$\rho(x) = \begin{cases} 
\beta & x \in (x_{i-1}, x_{i-1} + \delta_0/k), \\
0 & x \in (x_{i-1} + \delta_0/k, x_i - \delta_0/k), \\
\beta & x \in (x_i - \delta_0/k, x_i).
\end{cases}$$

(2.20)
Figure 2.1: An illustration of Krein’s theory in 1D: $[0, L]$; the first row shows the minimizers of $\lambda_1$ and $\lambda_2$, and the second row shows the maximizers of $\lambda_1$ and $\lambda_2$.

Several of the above arguments are still valid even in higher dimension when considering the domain $\Omega = B_R$, a ball of radius $R$. In particular, we have

**Theorem 2.3.7. (Krein)** Let $\Omega = B_R$ be a ball of radius $R$. Then
(i) The minimum of $\lambda_1(\rho)$ in the class $A$ defined in (2.8) is attained uniquely for the function $\rho_1$ given by

$$
\rho_1(x) = \begin{cases} 
\beta & \text{for } |x| \leq \delta, \\
\alpha & \text{for } \delta < |x| < R,
\end{cases}
$$

(2.21)

where $\delta$ is defined by the equality $(\beta - \alpha)|B_\delta| + \alpha|R| = c.$

(ii) The maximum of $\lambda_1(\rho)$ in the class $A$ is attained uniquely for the function $\rho^1$ given by

$$
\rho^1(x) = \begin{cases} 
\alpha & \text{for } |x| \leq \delta, \\
\beta & \text{for } \delta < |x| < R,
\end{cases}
$$

(2.22)

where $\delta$ is defined by the equality $(\alpha - \beta)|B_\delta| + \beta|R| = c.$

For a general case, given an open bounded connected set $\Omega \subset \mathbb{R}^n$, S.J. Cox and J.R. McLaughlin [13] showed that these extremizers vary continuously with respect to the proportion of the two constituents. They developed a geometric characterization of the extremizers in terms of the level sets of the corresponding eigenfunctions.

**Theorem 2.3.8. (Cox-McLaughlin)**

(i) Let $\rho_1$ be a minimizer of $\lambda_1(\rho)$ in the class $A$ defined in (2.8) and $u_1$ be the associated first eigenfunction. Then, there exists $l > 0$ such that, for each $x \in \Omega$,

$$
\rho_1(x) = \beta \implies u_1(x) \geq l,
$$

$$
\rho_1(x) = \alpha \implies u_1(x) \leq l,
$$

(2.23)
and $\rho_1 = \beta \chi_D + \alpha \chi_{\Omega \setminus D}$ where $D$ is the level set $D = \{x \in \Omega, u_1(x) \geq l\}$. (See Figure 2.2 for the minimizer of $\lambda_1$.)

(ii) Let $\rho^1$ be a maximizer of $\lambda_1(\rho)$ in the class $\mathcal{A}$ and $u^1$ be the associated first eigenfunction. Then, there exists $l > 0$ such that, for each $x \in \Omega$,

$$
\rho^1(x) = \beta \implies u_1(x) \leq l,
$$

$$
\rho^1(x) = \alpha \implies u_1(x) \geq l,
$$

and $\rho^1 = \beta \chi_D + \alpha \chi_{\Omega \setminus D}$ where $D$ is the level set $D = \{x \in \Omega, u_1(x) \leq l\}$.

Moreover, the maximizer is unique.

Figure 2.2: An illustration of Cox-McLaughlin’s theory of the minimizer of $\lambda_1$. 

16
Remark 2.3.9  Uniqueness of the maximizer comes immediately from the fact that $\rho \to 1/\lambda_1(\rho)$ is convex (Theorem 2.3.1). However, the uniqueness of the minimizer does not follow. Symmetry breaking phenomena is described in [10], which usually implies non-uniqueness. In particular, a dumbbell shaped domain under certain settings will give at least two minimizers, the complement of each optimal set is contained in one of the lobes.
CHAPTER 3

FORWARD PROBLEM FOR ELLIPTIC EIGENVALUE PROBLEMS

3.1 Numerical Methods

In the forward elliptic eigenvalue problem, the ability to update the density function iteratively to obtain the optimal configuration for eigenvalue optimization problems, depends on the ability to compute the eigenvalues and eigenfunctions of the elliptic eigenvalue problems for any given $\rho(x)$ efficiently and accurately. Many numerical techniques have been developed to solve the forward elliptic eigenvalue problems, e.g., the finite element method, the finite difference method, the spectral method and the boundary integral method. The finite element method is well suited for problems with complicated geometries while the finite difference method is often considered as the simplest method to learn and implement. This chapter provides the details of the implementation for these two types of methods.
3.1.1 Finite Element Method Formulation

A good starting point is to introduce the finite element method for one-dimensional (1D) problems with Dirichlet boundary condition. Then extend the method to two-dimensional (2D) problems where piecewise polynomial approximations are defined on triangulations of the spatial domain. Finally, formulate the method in 2D for general Robin boundary problems. For more general elliptic operators, see [36].

Dirichlet Problem in 1D

Consider the eigenvalue equation

\[-u'' = \lambda \rho u \quad \text{in} \quad \Omega = (0, 1),\]
\[u(0) = u(1) = 0,\]

where \( \rho = \rho(x) \) is a non-negative function, \( \lambda \) is the eigenvalue and \( u = u(x) \) is the corresponding eigenfunction. Recall the variational form of this problem is to find \( u \in H^1_0(\Omega) \) such that

\[k(u, \nu) = \lambda (\rho u, \nu), \quad \forall \nu \in H^1_0,\]

where

\[k(u, \nu) = \int_\Omega u' \nu' dx, \quad \text{and} \quad (\rho u, \nu) = \int_\Omega \rho u \nu dx.\]

To construct an approximate solution of (3.2), introduce the partition of the domain \([0, 1]\),

\[0 = x_0 < x_1 < \cdots < x_N = 1\]

where \( x_j = jh, \ j = 0, \cdots, N, \) and \( h = 1/N.\)
The discrete solution will then be solved in the finite-dimensional space of functions:

\[ V_h = \{ w \in C(\bar{\Omega}) : w \text{ is linear on each interval } [x_{j-1}, x_j], \ w(0) = w(1) = 0. \} \quad (3.5) \]

Define the hat functions \( \Phi_i \) as:

\[
\Phi_i(x_j) = \begin{cases} 
1 & \text{if } j = i, \\
0 & \text{if } j \neq i.
\end{cases}
\] (3.6)

Figure 3.1 illustrates several hat functions. It is quite obvious that the set \( \{ \Phi_i \}_{i=1}^{N-1} \subset V_h \) forms a basis for \( V_h \). Since globally the solution \( u^h \) is determined by its values at the grid points, it can be represented as

\[
u^h(x) = \sum_{j=1}^{N-1} U_j \Phi_j(x), \quad \text{with} \ U_j = u(x_j). \quad (3.7)\]
Now the finite-dimensional problem of solving $u^h \in V_h$ is

$$k(u^h, \Phi_i) = \lambda(\rho u^h, \Phi_i).$$  \hspace{1cm} (3.8)

Direct substituting of equation (3.7) gives the system of equations

$$\sum_{j=1}^{N-1} U_j k(\Phi_j, \Phi_i) = \lambda \sum_{j=1}^{N-1} U_j (\rho \Phi_j, \Phi_i), \quad \text{for } i = 1, \cdots N - 1.$$  \hspace{1cm} (3.9)

Using the notation:

$$K_{i,j} = \int_{\Omega} \Phi'_j(x)\Phi'_i(x)dx \quad \text{Stiffness matrix}, \hspace{1cm} (3.10)$$

$$M_{i,j} = \int_{\Omega} \rho(x)\Phi_j(x)\Phi_i(x)dx \quad \text{Mass matrix},$$

(3.9) becomes the generalized eigenvalue equation

$$KU = \lambda MU.$$  \hspace{1cm} (3.11)

This linear eigenvalue problem can be solved by the Arnoldi algorithm applied to a shifted and inverted matrix [5].

**Dirichlet Problem in 2D**

Now consider a domain $\Omega \in \mathcal{R}^2$ whose boundary $\Gamma$ is a polygon. The eigenvalue problem is

$$-\Delta u = \lambda \rho u \quad \text{in } \Omega,$$

$$u = 0 \quad \text{on } \Gamma.$$  \hspace{1cm} (3.12)

The variational form of this problem is to find $u \in H^1_0(\Omega)$ such that

$$k(u, \nu) = \lambda(\rho u, \nu), \quad \forall \nu \in H^1_0,$$  \hspace{1cm} (3.13)
where
\[ k(u, \nu) = \int_\Omega \nabla u \cdot \nabla \nu dx, \quad \text{and} \quad (\rho u, \nu) = \int_\Omega \rho u \nu dx. \quad (3.14) \]

The approximation of the solution follows similar lines as in the 1D case. This time the domain \( \Omega \) is covered by a triangular mesh, that is, \( \tau_h = \{ f_i \}_{i=1}^N \) is a triangulation of \( \Omega \) with faces \( f_1, \cdots, f_N \), such that
\[ \Omega = \bigcup_i f_i, \quad h_i = \text{diam} f_i, \quad h = \max_i h_i. \quad (3.15) \]

The associated function space \( V_h \) consists of continuous, piecewise linear functions on the triangular mesh \( \tau_h \), vanishing on the boundary \( \Gamma \), that is,
\[ V_h = \{ w \in C(\overline{\Omega}) : w \text{ is linear on each triangle } f_i \in \tau_h, \ w = 0 \text{ on } \Gamma. \} \quad (3.16) \]

Let \( P_1, \cdots, P_M \) be the interior vertices, that is, those that do not lie on \( \Gamma \). It is then obvious that a set of tent functions \( \{ \Phi_i \}_{i=1}^M \in V_h \) forms a basis for \( V_h \), where \( \Phi_i \) are defined as:
\[ \Phi_i(P_j) = \begin{cases} 1 & \text{if } j = i, \\ 0 & \text{if } j \neq i. \end{cases} \quad (3.17) \]

Figure 3.2 shows a tent function \( \Phi_i \) defined on the vertex \( P_i \). Any \( u \in V_h \) can be represented as
\[ u^h(x) = \sum_{j=1}^M U_j \Phi_j(x), \quad \text{with} \quad U_j = u(P_j). \quad (3.18) \]

It remains to solve the finite-dimensional problem
\[ k(u^h, \Phi_i) = \lambda(\rho u^h, \Phi_i). \quad (3.19) \]
Figure 3.2: A tent function in 2D

Direct substitution of equation (3.18) into (3.19) gives the system of equations

\[ \sum_{j=1}^{M} U_j k(\Phi_j, \Phi_i) = \lambda \sum_{j=1}^{M} U_j (\rho \Phi_j, \Phi_i), \quad \text{for } i = 1, \cdots M. \]  

(3.20)

This system can be expressed as

\[ KU = \lambda MU, \]  

(3.21)

where \( K, M \) are given by (3.10). Again, the Arnoldi algorithm is applied to a shifted and inverted matrix to solve this linear eigenvalue problem.

**General Robin Boundary Condition**

Next, consider the general Robin boundary problem:

\[-\Delta u = \lambda \rho u \quad \text{in} \quad \Omega, \]

\[ \partial_n u + \beta u = 0 \quad \text{on} \quad \Gamma. \]  

(3.22)
The weak form of the differential equation is obtained by multiplying the equation with an arbitrary test function \( \nu \) and integrating over \( \Omega \):
\[
\int_{\Omega} - (\Delta u) \nu \, dx = \int_{\Omega} \lambda \rho u \nu \, dx.
\] (3.23)

Green’s formula converts this statement into
\[
\int_{\Omega} \nabla u \cdot \nabla \nu \, dx - \int_{\partial \Omega} \frac{\partial u}{\partial n} \nu \, ds = \lambda \int_{\Omega} \rho u \nu \, dx.
\] (3.24)

The boundary condition (3.22) changes the boundary integral,
\[
\int_{\Omega} \nabla u \cdot \nabla \nu \, dx - \int_{\partial \Omega} (\beta u) \nu \, ds = \lambda \int_{\Omega} \rho u \nu \, dx.
\] (3.25)

An approximate solution to (3.25) can be constructed by using the triangulation (3.15) with vertices \( P_1, \cdots, P_{M_h} \), and projecting the weak form (3.25) of the differential equation onto a finite-dimensional subspace
\[
V_h = \{ w \in H^1 : w \text{ linear on each triangle } f_i \in \tau_h. \} \tag{3.26}
\]

By choosing the basis functions \( \{ \Phi_i \}_{i=1}^{M_h} \in V_h \) as the test functions, (3.25) becomes
\[
\int_{\Omega} \nabla u \cdot \nabla \Phi_i \, dx - \int_{\partial \Omega} (\beta u) \Phi_i \, ds = \lambda \int_{\Omega} \rho \Phi_i, \quad i = 1, \cdots, M_h.
\] (3.27)

Express the solution in the form
\[
u^h(x) = \sum_{j=1}^{M_h} U_j \Phi_j(x), \quad \text{with} \quad U_j = u(P_j), \tag{3.28}
\]

where to obtain the system of equations
\[
\sum_{j=1}^{M_h} \left( \int_{\Omega} \nabla \Phi_j \cdot \nabla \Phi_i \, dx + \int_{\partial \Omega} \beta \Phi_j \Phi_i \, ds \right) U_j = \lambda \sum_{j=1}^{M_h} \left( \int_{\Omega} \rho \Phi_j \Phi_i \right) U, \quad i = 1, \cdots, M_h.
\] (3.29)
Let

\[ B_{i,j} = \int_{\partial \Omega} \beta \Phi_j(x) \Phi_i(x) dx, \]
\[ M_{i,j} = \int_{\Omega} \rho(x) \Phi_j(x) \Phi_i(x) dx, \] (3.30)

then (3.29) is the generalized eigenvalue equation

\[ (K + B)U = \lambda MU, \] (3.31)

which can be solved efficiently.

### 3.1.2 Finite Difference Method Formulation

The finite difference method for the elliptic eigenvalue problems in 2D is based on using a rectangular mesh. Two cases will be considered, Dirichlet and general Robin boundary conditions. Please refer to [36] for more general elliptic operators.

**Dirichlet Problem**

Consider the problem (3.12) where the Laplace operator is

\[ \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}. \] (3.32)

Assume that \( \Omega \) is a square with a uniform mesh grid, that is, \( \Omega = [0,1] \times [0,1] \). Introduce \((M + 1) \times (M + 1)\) mesh points

\[ 0 = x_0 < x_1 < \cdots < x_M = 1, \quad 0 = y_0 < y_1 < \cdots < y_M = 1 \] (3.33)

by setting

\[ x_i = ih, \quad y_j = jh, \quad j = 0, \cdots, M, \]
\[ u_{i,j} = u(ih, jh), \] (3.34)
where \( h = 1/M \). By using the centered difference approximation for the derivatives,

\[
\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2},
\]

(3.35)

\[
\frac{\partial^2 u}{\partial y^2} \approx \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{h^2}.
\]

(3.36)

Figure 3.3 illustrates the 5-point stencil for Laplace operator. Substituting (3.35) and

(3.36) into equation (3.12) and after some re-arrangement,

\[
4u_{i,j} - (u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1}) = \lambda h^2 \rho_{i,j} u_{i,j}, \quad \text{for } i, j = 1, \cdots, M - 1,
\]

\[
u_{0,j} = u_{M,j} = u_{i,0} = u_{M,0} = 0.
\]

(3.37)

Thus our discrete problem may be written in the matrix form

\[
AU = \lambda BU,
\]

(3.38)

26
where $U = (u_{i,j})$, $B = (h^2 \rho_{ij})$. $A$ is a block tridiagonal $(M - 1) \times (M - 1)$ matrix. Then the Arnoldi algorithm can be applied to a shifted and inverted matrix to solve this generalized eigenvalue problem.

**General Robin Boundary Condition**

Consider the problem (3.22) with the general Robin boundary condition

$$\partial_n u + \beta u = 0.$$  

(3.39)

Approximate the derivatives along the boundary by introducing fictitious grid points outside the domain $\Omega$. The second-order central finite difference scheme applied to the first derivative, along the boundaries produces

$$\left. \frac{\partial u}{\partial x} \right|_{i=0} \approx \frac{u_{1,j} - u_{-1,j}}{2h}, \quad \left. \frac{\partial u}{\partial x} \right|_{i=M} \approx \frac{u_{M+1,j} - u_{M-1,j}}{2h},$$

$$\left. \frac{\partial u}{\partial y} \right|_{j=0} \approx \frac{u_{i,1} - u_{i,-1}}{2h}, \quad \left. \frac{\partial u}{\partial y} \right|_{j=M} \approx \frac{u_{i,M+1} - u_{i,M-1}}{2h}.$$  

(3.40)

(3.41)

Thus, the numerical approximation of problem (3.22) incorporating the boundary conditions becomes

$$4u_{i,j} - (u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1}) = \lambda h^2 \rho_{i,j} u_{i,j} \quad \text{for } i, j = 1, \cdots, M - 1,$n

$$(4 + 2h\beta)u_{0,j} - (2u_{1,j} + u_{0,j-1} + u_{0,j+1}) = \lambda h^2 \rho_{0,j} u_{0,j} \quad \text{at } i = 0,$n

$$(4 + 2h\beta)u_{M,j} - (2u_{M-1,j} + u_{M,j-1} + u_{M,j+1}) = \lambda h^2 \rho_{M,j} u_{M,j} \quad \text{at } i = M,$n

$$(4 + 2h\beta)u_{i,0} - (2u_{i,1} + u_{i-1,0} + u_{i+1,0}) = \lambda h^2 \rho_{i,0} u_{i,0} \quad \text{at } j = 0,$n

$$(4 + 2h\beta)u_{i,M} - (2u_{i,M-1} + u_{i-1,M} + u_{i+1,M}) = \lambda h^2 \rho_{i,M} u_{i,M} \quad \text{at } j = M.$$

(3.42)
Without too much difficulty, the discrete equations can be again written in the matrix form

$$AU = \lambda BU,$$  \hspace{1cm} (3.43)

where $U = (u_{i,j})$, $B = (h^2 \rho_{ij})$. $A$ is a block tridiagonal $(M - 1) \times (M - 1)$ matrix containing contributions from the boundary values. The Arnoldi algorithm can be applied to a shifted and inverted matrix to solve this generalized eigenvalue problem.

### 3.2 Tests of algorithms

In this section, tests of the accuracy of the forward problem solvers and the codes that implemented them are performed on known solutions for a unit square $\Omega = [0, 1] \times [0, 1]$. The solutions are constructed exactly for the different boundary conditions by the method of separation of variables and Appendix A contains the details. Here only a list of the positive eigenvalues and associated eigenfunctions are provided. A superscript $+$ is used to indicate positive eigenvalues.

1. Dirichlet Problem

   The problem

   $$-\Delta u(x, y) = \lambda u(x, y) \quad \Omega = [0, 1] \times [0, 1],$$

   $$u(x, y) = 0 \quad \partial \Omega,$$

   has the solutions

   $$u(x, y) = C \sin(k\pi x) \sin(l\pi y), \quad C \text{ is a constant}$$

   $$\lambda = (k\pi)^2 + (l\pi)^2, \quad k, l \in \mathbb{Z}.$$  \hspace{1cm} (3.45)
The first nine eigenvalues are

\[ \lambda_{1,9}^+ = (2, 5, 8, 10, 13, 17) \pi^2. \]  

(3.46)

2. Neumann Problem

The problem

\[-\Delta u(x, y) = \lambda u(x, y) \quad \Omega = [0, 1] \times [0, 1],\]
\[\partial u/\partial n = 0 \quad \partial \Omega,\]

has solutions

\[ u(x, y) = C \cos(k\pi x) \cos(l\pi y), \quad C \text{ is a constant} \]
\[\lambda = (k\pi)^2 + (l\pi)^2, \quad k, l \in \mathbb{Z}. \]

Thus the first nine positive eigenvalues are

\[ \lambda_{1,9}^+ = (1, 1, 2, 4, 4, 5, 8, 9) \pi^2. \]  

(3.49)

3. Robin Problem

The problem

\[-\Delta u(x, y) = \lambda u(x, y) \quad \Omega = [0, 1] \times [0, 1],\]
\[\partial u/\partial n + u = 0 \quad \partial \Omega,\]

has solutions

\[ u(x, y) = (C_1 \cos(\sqrt{\tau_1} x) + C_2 \sin(\sqrt{\tau_1} x))(C_3 \cos(\sqrt{\tau_2} y) + C_4 \sin(\sqrt{\tau_2} y)), \]
\[\lambda = \tau_1 + \tau_2, \]

(3.51)
where $C_1, C_2, C_3, C_4$ are constants, and $\tau_1, \tau_2$ are solutions of the equation

\[
f(\tau) = 2\sqrt{\tau} + (1 - \tau) \tan \sqrt{\tau} = 0.
\]

The first several solutions for the above nonlinear equation are

\[
\tau = 1.7071, 13.492, 43.357.
\]

Thus, the first nine eigenvalues are

\[
\begin{align*}
\lambda_1^+ &= 3.4141, & \lambda_4^+ &= 26.985, & \lambda_7^+ &= 56.850, \\
\lambda_2^+ &= 15.199, & \lambda_5^+ &= 45.064, & \lambda_8^+ &= 56.850, \\
\lambda_3^+ &= 15.199, & \lambda_6^+ &= 45.064, & \lambda_9^+ &= 86.714.
\end{align*}
\]

4. Dirichlet Problem with Variable Coefficient

The problem

\[
-\Delta u(x, y) = \lambda \rho(x) u(x, y) \quad \Omega = [0, 1] \times [0, 1],
\]

\[
u = 0 \quad \partial \Omega,
\]

where

\[
\rho(x) = \begin{cases} 
1 & x \in \left[0, \frac{1}{2}\right), \\
2 & x \in \left(\frac{1}{2}, 1\right],
\end{cases}
\]

has solutions of the form

\[
u(x, y) = T(x) S(y),
\]

where $S(y)$ is

\[
S = a_1 \sin(\sqrt{C}y), \quad a_1 \text{ constant}
\]

\[
C = (k\pi)^2, \quad k \in \mathbb{Z},
\]

\[
(3.57)
\]
and \( T(x) \) satisfies

\[
T'' + (\lambda - C)T = 0 \quad \text{in } (0, \frac{1}{2})
\]

\[
T'' + (2\lambda - C)T = 0 \quad \text{in } (\frac{1}{2}, 1)
\]

\[
T(0) = T(1) = 0.
\]

Assuming \( \lambda > 0 \) and \( T > 0 \), here are three possibilities:

(I) \( 2\lambda - C > \lambda - C > 0 \)

The equation for the eigenvalue is

\[
\frac{\tan \frac{\sqrt{\lambda-C}}{2}}{\tan \frac{\sqrt{2\lambda-C}}{2}} = -\frac{\sqrt{\lambda-C}}{\sqrt{2\lambda-C}}.
\]

(II) \( 2\lambda - C > 0 > \lambda - C \)

The equation for the eigenvalue is

\[
\frac{\tanh \frac{\sqrt{C-\lambda}}{2}}{\tanh \frac{\sqrt{2\lambda-C}}{2}} = -\frac{\sqrt{C-\lambda}}{\sqrt{2\lambda-C}}.
\]

(III) \( 0 > 2\lambda - C > \lambda - C \)

The equation for the eigenvalue is

\[
\frac{\tanh \frac{\sqrt{C-\lambda}}{2}}{\tanh \frac{\sqrt{C-2\lambda}}{2}} = -\frac{\sqrt{C-\lambda}}{\sqrt{C-2\lambda}}.
\]

Numerical solutions to these equations give the first nine eigenvalues

\[
\begin{align*}
\lambda_1^+ &= 12.516, & \lambda_4^+ &= 56.297, & \lambda_7^+ &= 86.964, \\
\lambda_2^+ &= 29.649, & \lambda_5^+ &= 58.265, & \lambda_8^+ &= 91.737, \\
\lambda_3^+ &= 35.976, & \lambda_6^+ &= 65.541, & \lambda_9^+ &= 92.225.
\end{align*}
\]
5. Neumann Problem with Variable Coefficient

The problem

\[-\Delta u(x, y) = \lambda \rho(x)u(x, y) \quad \Omega = [0, 1] \times [0, 1], \]
\[
\frac{\partial u}{\partial n} = 0 \quad \partial \Omega,
\]

where

\[
\rho(x) = \begin{cases} 
1 & x \in [0, \frac{1}{2}), \\
2 & x \in (\frac{1}{2}, 1], 
\end{cases}
\]

has the solution \( u(x, y) = T(x)S(y), \) where

\[
S = a_1 \cos(\sqrt{C}y), \quad a_1 \text{ constant}
\]
\[
C = (k\pi)^2, \quad k \in \mathbb{Z},
\]

and \( T(x) \) satisfies

\[
T'' + (\lambda - C)T = 0 \quad \text{in } (0, \frac{1}{2})
\]
\[
T'' + (2\lambda - C)T = 0 \quad \text{in } (\frac{1}{2}, 1)
\]
\[
T'(0) = T'(1) = 0.
\]

Assuming \( \lambda > 0 \) and \( T > 0 \), here are three possibilities

(I) \( 2\lambda - C > \lambda - C > 0 \)

The equation for the eigenvalue is

\[
\sqrt{\lambda - C} \tan \frac{\sqrt{\lambda - C}}{2} + \sqrt{2\lambda - C} \tan \frac{\sqrt{2\lambda - C}}{2} = 0. \quad (3.67)
\]

(II) \( 2\lambda - C > 0 > \lambda - C \)

The equation for the eigenvalue is

\[
\sqrt{C - \lambda} \tanh \frac{\sqrt{C - \lambda}}{2} - \sqrt{2\lambda - C} \tan \frac{\sqrt{2\lambda - C}}{2} = 0. \quad (3.68)
\]
(III) \[ 0 > 2\lambda - C > \lambda - C \]

The equation for the eigenvalue is

\[
\sqrt{C - \lambda} \tanh \frac{\sqrt{C - \lambda}}{2} + \sqrt{C - 2\lambda} \tan \frac{\sqrt{C - 2\lambda}}{2} = 0. \quad (3.69)
\]

Numerical solutions to these equations give the first nine positive eigenvalues

\[
\begin{align*}
\lambda_1^+ &= 6.0967, \quad \lambda_4^+ = 22.073, \quad \lambda_7^+ = 39.478, \\
\lambda_2^+ &= 7.1691, \quad \lambda_5^+ = 25.819, \quad \lambda_8^+ = 47.343, \\
\lambda_3^+ &= 15.273, \quad \lambda_6^+ = 32.312, \quad \lambda_9^+ = 53.531. \quad (3.70)
\end{align*}
\]

6. Robin Problem with Variable Coefficient

The problem

\[
\begin{align*}
-\Delta u(x, y) &= \lambda \rho(x) u(x, y) \quad \Omega = [0, 1] \times [0, 1], \\
\frac{\partial u}{\partial n} + u &= 0 \quad \partial \Omega,
\end{align*}
\]

where

\[
\rho(x) = \begin{cases}
1 & x \in [0, \frac{1}{2}), \\
2 & x \in (\frac{1}{2}, 1],
\end{cases}
\]

has the solution \( u(x, y) = T(x)S(y) \), where

\[
S = a_1 \cos \sqrt{C}y + a_2 \sin \sqrt{C}y, \quad a_1, a_2 \text{ are constants,}
\]

where \( C \) is the solution of the equation

\[
f(\tau) = 2\sqrt{\tau} + (1 - \tau) \tan \sqrt{\tau} = 0. \quad (3.74)
\]
The first several solutions for the above nonlinear equation are

$$\tau = 1.7071, 13.492, 43.357, 92.769.$$  (3.75)

The function $T(x)$ satisfies

$$T'' + (\lambda - C)T = 0 \quad \text{in } (0, \frac{1}{2})$$
$$T'' + (2\lambda - C)T = 0 \quad \text{in } (\frac{1}{2}, 1)$$

$$T(0) - T'(0) = 0$$
$$T(1) + T'(1) = 0.$$  (3.76)

Assuming $\lambda > 0$ and $T > 0$, there are three possibilities:

(I) $2\lambda - C > \lambda - C > 0$

The equation for the eigenvalue is

$$\frac{\sqrt{\lambda-C} \cos \frac{\sqrt{\lambda-C}}{2} + \sin \frac{\sqrt{\lambda-C}}{2}}{(\lambda-C) \sin \frac{\sqrt{\lambda-C}}{2} - \sqrt{\lambda-C} \cos \frac{\sqrt{\lambda-C}}{2}} + \frac{\sqrt{2\lambda-C} \cos \frac{\sqrt{2\lambda-C}}{2} + \sin \frac{\sqrt{2\lambda-C}}{2}}{(2\lambda-C) \sin \frac{\sqrt{2\lambda-C}}{2} - \sqrt{2\lambda-C} \cos \frac{\sqrt{2\lambda-C}}{2}} = 0.$$  (3.77)

(II) $2\lambda - C > 0 > \lambda - C$

The equation for the eigenvalue is

$$\frac{\sqrt{\lambda-C} \cosh \frac{\sqrt{\lambda-C}}{2} + \sinh \frac{\sqrt{\lambda-C}}{2}}{(\lambda-C) \sinh \frac{\sqrt{\lambda-C}}{2} + \sqrt{\lambda-C} \cosh \frac{\sqrt{\lambda-C}}{2}} + \frac{\sqrt{2\lambda-C} \cosh \frac{\sqrt{2\lambda-C}}{2} + \sinh \frac{\sqrt{2\lambda-C}}{2}}{-(2\lambda-C) \sinh \frac{\sqrt{2\lambda-C}}{2} + \sqrt{2\lambda-C} \cosh \frac{\sqrt{2\lambda-C}}{2}} = 0.$$  (3.78)

(III) $0 > 2\lambda - C > \lambda - C$

The equation for the eigenvalue is

$$\frac{\sqrt{\lambda-C} \cosh \frac{\sqrt{\lambda-C}}{2} + \sinh \frac{\sqrt{\lambda-C}}{2}}{(\lambda-C) \sinh \frac{\sqrt{\lambda-C}}{2} + \sqrt{\lambda-C} \cosh \frac{\sqrt{\lambda-C}}{2}} + \frac{\sqrt{2\lambda-C} \cosh \frac{\sqrt{2\lambda-C}}{2} + \sinh \frac{\sqrt{2\lambda-C}}{2}}{(C-2\lambda) \sin \frac{\sqrt{2\lambda-C}}{2} + \sqrt{2\lambda-C} \cosh \frac{\sqrt{2\lambda-C}}{2}} = 0.$$  (3.79)
Numerical solutions to these equations give the first nine eigenvalues

\[ \lambda_1^+ = 2.2206, \quad \lambda_4^+ = 20.837, \quad \lambda_7^+ = 37.560, \]
\[ \lambda_2^+ = 9.2533, \quad \lambda_5^+ = 25.327, \quad \lambda_8^+ = 44.102, \]
\[ \lambda_3^+ = 11.197, \quad \lambda_6^+ = 29.614, \quad \lambda_9^+ = 50.715. \]  

(3.80)

3.2.1 Accuracy Test for the Finite Element Method

The PDE Toolbox in MATLAB allows an easy way to test the finite element method on a triangulated mesh. (Figure 3.4 gives an example of a triangulated mesh with a maximum edge length 0.375.) Subsequently, all edges of each triangle are divided in half and the process repeated \( Nr \) times. Let \( hr \) be the ratio of the lengths of each edge to the initial mesh, and \( \lambda_k^h \) be the numerical solutions of eigenvalues. Figure 3.5 illustrates the results of the finite element method applied to the Dirichlet boundary problem. A table of errors in eigenvalues is given in Table 3.1. We can see that the numerically determined eigenvalues converge to the exact eigenvalues from above and the order of convergence is two. Similar results for the Neumann and Robin boundary problems are presented in Table 3.2 and 3.3, respectively. Once again the finite element method is \( \mathcal{O}(h^2) \) as expected. Tests are also conducted for variable densities and the results for the Dirichlet, Neumann, and Robin boundary problems are shown in Table 3.4, 3.5, and 3.6 respectively. As we can observe from the table of errors, the finite element method is \( \mathcal{O}(h^2) \). For simplicity, the superscript + will be omitted and \( \lambda_k, \ k = 1, \cdots, 9 \) will denote the first nine eigenvalues throughout the whole paper.
Figure 3.4: The triangulated mesh with a maximum edge length 0.375.
Figure 3.5: Results of the application of the finite element method to the Dirichlet problem. Left panel shows the first 9 eigenvalues for different mesh sizes, and the right panel plots $\log(\lambda^h_k - \lambda_k)$ vs. $\log(h)$. 
<table>
<thead>
<tr>
<th>Nr</th>
<th>$hr$</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
<th>$\lambda_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$2^{-2}$</td>
<td>1.8669e-001</td>
<td>1.0263e+000</td>
<td>1.0263e+000</td>
<td>2.1249e+000</td>
</tr>
<tr>
<td>3</td>
<td>$2^{-3}$</td>
<td>4.7263e-002</td>
<td>2.5983e-001</td>
<td>2.5983e-001</td>
<td>5.4797e-001</td>
</tr>
<tr>
<td>4</td>
<td>$2^{-4}$</td>
<td>1.9822</td>
<td>1.9983</td>
<td>1.9983</td>
<td>2.0055</td>
</tr>
</tbody>
</table>

Table 3.1: Errors in the eigenvalues determined by the finite element method applied to the Dirichlet problem.
<table>
<thead>
<tr>
<th>$Nr$</th>
<th>$hr$</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
<th>$\lambda_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$2^{-2}$</td>
<td>3.0756e-002</td>
<td>3.0756e-002</td>
<td>1.8669e-001</td>
<td>4.9389e-001</td>
</tr>
<tr>
<td>3</td>
<td>$2^{-3}$</td>
<td>7.8484e-003</td>
<td>7.8484e-003</td>
<td>4.7263e-002</td>
<td>1.2567e-001</td>
</tr>
<tr>
<td>4</td>
<td>$2^{-4}$</td>
<td>1.9757e-003</td>
<td>1.9757e-003</td>
<td>1.1867e-002</td>
<td>3.1617e-002</td>
</tr>
<tr>
<td>5</td>
<td>$2^{-5}$</td>
<td>4.9500e-004</td>
<td>4.9500e-004</td>
<td>2.9709e-003</td>
<td>7.9203e-003</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.9862</td>
<td>1.9862</td>
<td>1.9915</td>
<td>1.9878</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$hr$</th>
<th>$\lambda_5$</th>
<th>$\lambda_6$</th>
<th>$\lambda_7$</th>
<th>$\lambda_8$</th>
<th>$\lambda_9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^{-2}$</td>
<td>4.9389e-001</td>
<td>1.0263e+000</td>
<td>1.0263e+000</td>
<td>2.1249e+000</td>
<td>2.5146e+000</td>
</tr>
<tr>
<td>$2^{-3}$</td>
<td>1.2567e-001</td>
<td>2.5983e-001</td>
<td>2.5983e-001</td>
<td>5.4797e-001</td>
<td>6.3698e-001</td>
</tr>
<tr>
<td>$2^{-4}$</td>
<td>3.1617e-002</td>
<td>6.5259e-002</td>
<td>6.5259e-002</td>
<td>1.3831e-001</td>
<td>1.6011e-001</td>
</tr>
<tr>
<td>$2^{-5}$</td>
<td>7.9203e-003</td>
<td>1.6339e-002</td>
<td>1.6339e-002</td>
<td>3.4673e-002</td>
<td>4.0099e-002</td>
</tr>
<tr>
<td></td>
<td>1.9878</td>
<td>1.9912</td>
<td>1.9912</td>
<td>1.9798</td>
<td>1.9904</td>
</tr>
</tbody>
</table>

Table 3.2: Errors in the eigenvalues determined by the finite element method applied to the Neumann problem.
<table>
<thead>
<tr>
<th>$N_r$</th>
<th>$hr$</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
<th>$\lambda_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$2^{-1}$</td>
<td>6.4312e-003</td>
<td>2.2869e-001</td>
<td>2.2869e-001</td>
<td>9.2598e-001</td>
</tr>
<tr>
<td>2</td>
<td>$2^{-2}$</td>
<td>1.7988e-003</td>
<td>6.0844e-002</td>
<td>6.0844e-002</td>
<td>2.4178e-001</td>
</tr>
<tr>
<td>3</td>
<td>$2^{-3}$</td>
<td>4.7293e-004</td>
<td>1.5871e-002</td>
<td>1.5871e-002</td>
<td>6.1318e-002</td>
</tr>
<tr>
<td>4</td>
<td>$2^{-4}$</td>
<td>1.2427e-004</td>
<td>4.3053e-003</td>
<td>4.3053e-003</td>
<td>1.5208e-002</td>
</tr>
</tbody>
</table>

| order | 1.9008 | 1.9132 | 1.9132 | 1.9764 |

<table>
<thead>
<tr>
<th>$hr$</th>
<th>$\lambda_5$</th>
<th>$\lambda_6$</th>
<th>$\lambda_7$</th>
<th>$\lambda_8$</th>
<th>$\lambda_9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^{-1}$</td>
<td>2.4363e+000</td>
<td>2.4365e+000</td>
<td>4.8740e+000</td>
<td>4.8740e+000</td>
<td>8.4206e+000</td>
</tr>
<tr>
<td>$2^{-2}$</td>
<td>6.3031e-001</td>
<td>6.3119e-001</td>
<td>1.2539e+000</td>
<td>1.2539e+000</td>
<td>2.3544e+000</td>
</tr>
<tr>
<td>$2^{-3}$</td>
<td>1.6042e-001</td>
<td>1.6073e-001</td>
<td>3.1728e-001</td>
<td>3.1728e-001</td>
<td>6.0886e-001</td>
</tr>
<tr>
<td>$2^{-4}$</td>
<td>4.0548e-002</td>
<td>4.0635e-002</td>
<td>7.9379e-002</td>
<td>7.9379e-002</td>
<td>1.5408e-001</td>
</tr>
</tbody>
</table>

| order | 1.9701 | 1.9691 | 1.9803 | 1.9803 | 1.9268 |

Table 3.3: Errors in the eigenvalues determined by the finite element method applied to the Robin problem.
<table>
<thead>
<tr>
<th>$Nr$</th>
<th>$hr$</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
<th>$\lambda_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$2^{-2}$</td>
<td>1.3075e-001</td>
<td>6.3414e-001</td>
<td>7.8038e-001</td>
<td>2.5155e+000</td>
</tr>
<tr>
<td>3</td>
<td>$2^{-3}$</td>
<td>3.3085e-002</td>
<td>1.6124e-001</td>
<td>1.9860e-001</td>
<td>6.3398e-001</td>
</tr>
<tr>
<td>4</td>
<td>$2^{-4}$</td>
<td>8.3030e-003</td>
<td>4.0510e-002</td>
<td>4.9924e-002</td>
<td>1.5904e-001</td>
</tr>
<tr>
<td>5</td>
<td>$2^{-5}$</td>
<td>2.0754e-003</td>
<td>1.0114e-002</td>
<td>1.2470e-002</td>
<td>3.9793e-002</td>
</tr>
<tr>
<td></td>
<td>order</td>
<td>1.9926</td>
<td>1.9904</td>
<td>1.9895</td>
<td>1.9942</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$hr$</th>
<th>$\lambda_5$</th>
<th>$\lambda_6$</th>
<th>$\lambda_7$</th>
<th>$\lambda_8$</th>
<th>$\lambda_9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^{-2}$</td>
<td>2.1916e+000</td>
<td>2.6198e+000</td>
<td>4.6929e+000</td>
<td>6.6965e+000</td>
<td>6.6493e+000</td>
</tr>
<tr>
<td>$2^{-3}$</td>
<td>5.6357e-001</td>
<td>6.5527e-001</td>
<td>1.1707e+000</td>
<td>1.6973e+000</td>
<td>1.6489e+000</td>
</tr>
<tr>
<td>$2^{-4}$</td>
<td>1.4215e-001</td>
<td>1.6408e-001</td>
<td>2.9286e-001</td>
<td>4.2645e-001</td>
<td>4.1161e-001</td>
</tr>
<tr>
<td>$2^{-5}$</td>
<td>3.5656e-002</td>
<td>4.1065e-002</td>
<td>7.3257e-002</td>
<td>1.0675e-001</td>
<td>1.0284e-001</td>
</tr>
<tr>
<td></td>
<td>order</td>
<td>1.9812</td>
<td>1.9984</td>
<td>2.0003</td>
<td>1.9906</td>
</tr>
</tbody>
</table>

Table 3.4: Errors in the eigenvalues determined by the finite element method applied to the Dirichlet problem with variable coefficient.
<table>
<thead>
<tr>
<th>$Nr$</th>
<th>$hr$</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
<th>$\lambda_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$2^{-2}$</td>
<td>2.3976e-002</td>
<td>2.3230e-002</td>
<td>1.4100e-001</td>
<td>3.5547e-001</td>
</tr>
<tr>
<td>3</td>
<td>$2^{-3}$</td>
<td>6.1226e-003</td>
<td>5.9588e-003</td>
<td>3.5783e-002</td>
<td>9.0181e-002</td>
</tr>
<tr>
<td>4</td>
<td>$2^{-4}$</td>
<td>1.5552e-003</td>
<td>1.5256e-003</td>
<td>9.0065e-003</td>
<td>2.2667e-002</td>
</tr>
<tr>
<td>5</td>
<td>$2^{-5}$</td>
<td>4.0446e-004</td>
<td>4.0744e-004</td>
<td>2.2714e-003</td>
<td>5.6789e-003</td>
</tr>
</tbody>
</table>

| order | 1.9645 | 1.9465 | 1.9858 | 1.9896 |

<table>
<thead>
<tr>
<th>$hr$</th>
<th>$\lambda_5$</th>
<th>$\lambda_6$</th>
<th>$\lambda_7$</th>
<th>$\lambda_8$</th>
<th>$\lambda_9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^{-2}$</td>
<td>3.5940e-001</td>
<td>7.2036e-001</td>
<td>7.7357e-001</td>
<td>1.5490e+000</td>
<td>1.6945e+000</td>
</tr>
<tr>
<td>$2^{-3}$</td>
<td>9.1244e-002</td>
<td>1.8208e-001</td>
<td>1.9953e-001</td>
<td>3.9179e-001</td>
<td>4.3047e-001</td>
</tr>
<tr>
<td>$2^{-4}$</td>
<td>2.2948e-002</td>
<td>4.5695e-002</td>
<td>5.0383e-002</td>
<td>9.8412e-002</td>
<td>1.0818e-001</td>
</tr>
<tr>
<td>$2^{-5}$</td>
<td>5.7567e-003</td>
<td>1.1426e-002</td>
<td>1.2645e-002</td>
<td>2.4635e-002</td>
<td>2.7082e-002</td>
</tr>
</tbody>
</table>

| order | 1.9884 | 1.993 | 1.979 | 1.9917 | 1.9895 |

Table 3.5: Errors in the eigenvalues determined by the finite element method applied to the Neumann problem with variable coefficient.
<table>
<thead>
<tr>
<th>$N_r$</th>
<th>$hr$</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
<th>$\lambda_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$2^{-1}$</td>
<td>5.1882e-003</td>
<td>1.6608e-001</td>
<td>1.7707e-001</td>
<td>7.6626e-001</td>
</tr>
<tr>
<td>2</td>
<td>$2^{-2}$</td>
<td>1.4079e-003</td>
<td>4.3875e-002</td>
<td>4.7388e-002</td>
<td>2.0251e-001</td>
</tr>
<tr>
<td>3</td>
<td>$2^{-3}$</td>
<td>3.4372e-004</td>
<td>1.1237e-002</td>
<td>1.2441e-002</td>
<td>5.1886e-002</td>
</tr>
<tr>
<td>4</td>
<td>$2^{-4}$</td>
<td>6.5497e-005</td>
<td>2.8581e-003</td>
<td>3.4381e-003</td>
<td>1.3263e-002</td>
</tr>
<tr>
<td></td>
<td>order</td>
<td>2.0957</td>
<td>1.9547</td>
<td>1.8989</td>
<td>1.9522</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$hr$</th>
<th>$\lambda_5$</th>
<th>$\lambda_6$</th>
<th>$\lambda_7$</th>
<th>$\lambda_8$</th>
<th>$\lambda_9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2^{-1}$</td>
<td>1.7289e+000</td>
<td>1.7715e+000</td>
<td>3.3490e+000</td>
<td>3.4398e+000</td>
<td>6.6646e+000</td>
</tr>
<tr>
<td>$2^{-2}$</td>
<td>4.4492e-001</td>
<td>4.5446e-001</td>
<td>8.5587e-001</td>
<td>9.5109e-001</td>
<td>1.6886e+000</td>
</tr>
<tr>
<td>$2^{-3}$</td>
<td>1.1300e-001</td>
<td>1.1490e-001</td>
<td>2.1638e-001</td>
<td>2.4609e-001</td>
<td>4.2685e-001</td>
</tr>
<tr>
<td>$2^{-4}$</td>
<td>2.8602e-002</td>
<td>2.8532e-002</td>
<td>5.4375e-002</td>
<td>6.2422e-002</td>
<td>1.0734e-001</td>
</tr>
<tr>
<td></td>
<td>order</td>
<td>1.973</td>
<td>1.9853</td>
<td>1.9818</td>
<td>1.9303</td>
</tr>
</tbody>
</table>

Table 3.6: Errors in the eigenvalues determined by the finite element method applied to the Robin problem with variable coefficient.
3.2.2 Accuracy Test for Finite Difference Method

In this subsection, tests are conducted on the accuracy of the finite difference method solver applied on equally spaced grids covering the unit square, i.e., rectangular meshes. Under refinement, all edges of each square are divided in half. Let $N$ be the number of subsquares in each dimension, $h$ be the grid spacing in each dimension, and $\lambda_k^h$ be the numerical solutions of eigenvalues. Figure 3.6 and Table 3.7 illustrate the results of applying the finite difference to the Dirichlet boundary problem. The eigenvalues converge to the exact eigenvalues from above and the order of convergence is two. Table 3.8 and 3.9 give the errors in the eigenvalues for the Neumann and Robin boundary problems. Once again the finite difference method is $O(h^2)$. Table 3.10, 3.11, and 3.12 give the errors for the Dirichlet, Neumann, and Robin boundary problems when the density varies. The finite difference method is still $O(h^2)$. 
Figure 3.6: Results of the application of the finite difference method to the Dirichlet problem. Left panel shows the first 9 eigenvalues for different mesh sizes, and the right panel plots $\log(\lambda^h_k - \lambda_k)$ vs. $\log(h)$. 
<table>
<thead>
<tr>
<th>( N )</th>
<th>( h )</th>
<th>( \lambda_1 )</th>
<th>( \lambda_2 )</th>
<th>( \lambda_3 )</th>
<th>( \lambda_4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>3.1250e-002</td>
<td>1.5849e-002</td>
<td>1.3460e-001</td>
<td>1.3460e-001</td>
<td>2.5334e-001</td>
</tr>
<tr>
<td>128</td>
<td>7.8125e-003</td>
<td>9.9088e-004</td>
<td>8.4220e-003</td>
<td>8.4220e-003</td>
<td>1.5853e-002</td>
</tr>
<tr>
<td>256</td>
<td>3.9063e-003</td>
<td>2.4772e-004</td>
<td>2.1056e-003</td>
<td>2.1056e-003</td>
<td>3.9635e-003</td>
</tr>
<tr>
<td></td>
<td>order</td>
<td>1.9999</td>
<td>1.9994</td>
<td>1.9994</td>
<td>1.9994</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( N )</th>
<th>( \lambda_5 )</th>
<th>( \lambda_6 )</th>
<th>( \lambda_7 )</th>
<th>( \lambda_8 )</th>
<th>( \lambda_9 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>6.4817e-001</td>
<td>6.4817e-001</td>
<td>7.6692e-001</td>
<td>7.6692e-001</td>
<td>2.0269e+000</td>
</tr>
<tr>
<td>64</td>
<td>1.6239e-001</td>
<td>1.6239e-001</td>
<td>1.9211e-001</td>
<td>1.9211e-001</td>
<td>5.0867e-001</td>
</tr>
<tr>
<td></td>
<td>order</td>
<td>1.9987</td>
<td>1.9987</td>
<td>1.9988</td>
<td>1.9988</td>
</tr>
</tbody>
</table>

Table 3.7: Errors in the eigenvalues determined by the finite difference method applied to the Dirichlet problem.
<table>
<thead>
<tr>
<th>$N$</th>
<th>$h$</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
<th>$\lambda_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>1.0000e-02</td>
<td>8.0351e-004</td>
<td>8.0351e-004</td>
<td>1.6325e-003</td>
<td>1.3076e-002</td>
</tr>
<tr>
<td>150</td>
<td>6.6667e-03</td>
<td>3.8252e-004</td>
<td>3.8252e-004</td>
<td>7.2515e-004</td>
<td>6.0804e-003</td>
</tr>
<tr>
<td>200</td>
<td>5.0000e-03</td>
<td>2.0352e-004</td>
<td>2.0352e-004</td>
<td>3.9662e-004</td>
<td>3.4431e-003</td>
</tr>
<tr>
<td>250</td>
<td>4.0000e-03</td>
<td>1.3082e-004</td>
<td>1.3082e-004</td>
<td>2.6365e-004</td>
<td>2.1520e-003</td>
</tr>
</tbody>
</table>

| order | 1.9806 | 1.9806 | 1.99  | 1.9508 |

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\lambda_5$</th>
<th>$\lambda_6$</th>
<th>$\lambda_7$</th>
<th>$\lambda_8$</th>
<th>$\lambda_9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>1.2382e-002</td>
<td>1.3884e-002</td>
<td>1.3242e-002</td>
<td>2.6568e-002</td>
<td>6.7555e-002</td>
</tr>
<tr>
<td>150</td>
<td>5.5572e-003</td>
<td>6.3937e-003</td>
<td>6.0478e-003</td>
<td>1.1676e-002</td>
<td>2.9766e-002</td>
</tr>
<tr>
<td>250</td>
<td>2.1251e-003</td>
<td>2.2257e-003</td>
<td>2.1999e-003</td>
<td>4.1960e-003</td>
<td>1.0660e-002</td>
</tr>
</tbody>
</table>

| order | 1.9149 | 1.9882 | 1.9363 | 2.0111 | 2.0039 |

Table 3.8: Errors in the eigenvalues determined by the finite difference method applied to the Neumann problem.
<table>
<thead>
<tr>
<th>$N$</th>
<th>$h$</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
<th>$\lambda_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>1.2500e-001</td>
<td>6.9906e-003</td>
<td>1.5372e-001</td>
<td>1.5372e-001</td>
<td>3.1554e-001</td>
</tr>
<tr>
<td>32</td>
<td>3.1250e-002</td>
<td>3.5964e-004</td>
<td>7.5371e-003</td>
<td>7.5371e-003</td>
<td>1.6534e-002</td>
</tr>
<tr>
<td>64</td>
<td>1.5625e-002</td>
<td>9.1563e-005</td>
<td>1.5150e-003</td>
<td>1.5150e-003</td>
<td>4.2215e-003</td>
</tr>
</tbody>
</table>

| order | 1.9744 | 2.0968 | 2.0968 | 1.9652 |

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\lambda_5$</th>
<th>$\lambda_6$</th>
<th>$\lambda_7$</th>
<th>$\lambda_8$</th>
<th>$\lambda_9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>2.5685e+000</td>
<td>2.5685e+000</td>
<td>2.7303e+000</td>
<td>2.7303e+000</td>
<td>5.1440e+000</td>
</tr>
<tr>
<td>16</td>
<td>5.7157e-001</td>
<td>5.7157e-001</td>
<td>6.0766e-001</td>
<td>6.0766e-001</td>
<td>1.1448e+000</td>
</tr>
<tr>
<td>32</td>
<td>1.3424e-001</td>
<td>1.3424e-001</td>
<td>1.4323e-001</td>
<td>1.4323e-001</td>
<td>2.6894e-001</td>
</tr>
</tbody>
</table>

| order | 1.9915 | 1.9915 | 1.9832 | 1.9832 | 1.9908 |

Table 3.9: Errors in the eigenvalues determined by the finite difference method applied to the Robin problem.
<table>
<thead>
<tr>
<th>$N$</th>
<th>$h$</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
<th>$\lambda_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>3.1250e-02</td>
<td>1.5037e-02</td>
<td>9.9307e-02</td>
<td>1.0303e-01</td>
<td>4.0645e-01</td>
</tr>
<tr>
<td>64</td>
<td>1.5625e-02</td>
<td>3.6450e-03</td>
<td>2.4110e-02</td>
<td>2.4995e-02</td>
<td>9.8698e-02</td>
</tr>
<tr>
<td>128</td>
<td>7.8125e-03</td>
<td>9.0007e-04</td>
<td>5.9665e-03</td>
<td>6.1871e-03</td>
<td>2.4320e-02</td>
</tr>
<tr>
<td>256</td>
<td>3.9063e-03</td>
<td>2.2633e-04</td>
<td>1.5114e-03</td>
<td>1.5700e-03</td>
<td>6.0496e-03</td>
</tr>
<tr>
<td></td>
<td>order</td>
<td>1.9917</td>
<td>1.9867</td>
<td>1.9861</td>
<td>1.9968</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\lambda_5$</th>
<th>$\lambda_6$</th>
<th>$\lambda_7$</th>
<th>$\lambda_8$</th>
<th>$\lambda_9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>2.3615e-01</td>
<td>5.3259e-01</td>
<td>6.1675e-01</td>
<td>7.3318e-01</td>
<td>1.1772e+00</td>
</tr>
<tr>
<td>64</td>
<td>5.7131e-02</td>
<td>1.2918e-01</td>
<td>1.4968e-01</td>
<td>1.7795e-01</td>
<td>2.8633e-01</td>
</tr>
<tr>
<td>128</td>
<td>1.4031e-02</td>
<td>3.1783e-02</td>
<td>3.6842e-02</td>
<td>4.3843e-02</td>
<td>7.0568e-02</td>
</tr>
<tr>
<td>256</td>
<td>3.4535e-03</td>
<td>7.8650e-03</td>
<td>9.1269e-03</td>
<td>1.0906e-02</td>
<td>1.7541e-02</td>
</tr>
<tr>
<td></td>
<td>order</td>
<td>2.0048</td>
<td>2.0003</td>
<td>1.9994</td>
<td>1.9971</td>
</tr>
</tbody>
</table>

Table 3.10: Errors in the eigenvalues determined by the finite difference method applied to the Dirichlet problem with variable coefficient.
<table>
<thead>
<tr>
<th>$N$</th>
<th>$h$</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
<th>$\lambda_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>1.0000e-002</td>
<td>5.6636e-004</td>
<td>4.8340e-004</td>
<td>1.0248e-003</td>
<td>8.2570e-003</td>
</tr>
<tr>
<td>150</td>
<td>6.6667e-003</td>
<td>2.2151e-004</td>
<td>2.3065e-004</td>
<td>5.5785e-004</td>
<td>3.0964e-003</td>
</tr>
<tr>
<td>200</td>
<td>5.0000e-003</td>
<td>1.1812e-004</td>
<td>1.0205e-004</td>
<td>2.7925e-004</td>
<td>1.8157e-003</td>
</tr>
<tr>
<td>250</td>
<td>4.0000e-003</td>
<td>6.7806e-005</td>
<td>5.1334e-005</td>
<td>1.6203e-004</td>
<td>1.0571e-003</td>
</tr>
</tbody>
</table>

| order | 2.286 | 2.4269 | 2.0046 | 2.1976 |

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\lambda_5$</th>
<th>$\lambda_6$</th>
<th>$\lambda_7$</th>
<th>$\lambda_8$</th>
<th>$\lambda_9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>1.3101e-002</td>
<td>1.0729e-002</td>
<td>1.2991e-002</td>
<td>3.4611e-002</td>
<td>2.1192e-002</td>
</tr>
<tr>
<td>150</td>
<td>4.5936e-003</td>
<td>5.2009e-003</td>
<td>5.8412e-003</td>
<td>1.5577e-002</td>
<td>9.2935e-003</td>
</tr>
<tr>
<td>200</td>
<td>2.5872e-003</td>
<td>2.9207e-003</td>
<td>3.3861e-003</td>
<td>8.6904e-003</td>
<td>5.3918e-003</td>
</tr>
<tr>
<td>250</td>
<td>1.6448e-003</td>
<td>1.8678e-003</td>
<td>2.0794e-003</td>
<td>5.5158e-003</td>
<td>3.3623e-003</td>
</tr>
</tbody>
</table>

| order | 2.2438 | 1.897  | 1.9721 | 1.9911 | 1.9843 |

Table 3.11: Errors in the eigenvalues determined by the finite difference method applied to the Neumann problem with variable coefficient.
<table>
<thead>
<tr>
<th>$N$</th>
<th>$h$</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
<th>$\lambda_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>1.2500e-001</td>
<td>1.1742e-002</td>
<td>6.7450e-002</td>
<td>1.5304e-001</td>
<td>4.4635e-001</td>
</tr>
<tr>
<td>16</td>
<td>6.2500e-002</td>
<td>2.9584e-003</td>
<td>1.6801e-002</td>
<td>3.7747e-002</td>
<td>1.0972e-001</td>
</tr>
<tr>
<td>64</td>
<td>1.5625e-002</td>
<td>2.1186e-004</td>
<td>1.0137e-003</td>
<td>1.9757e-003</td>
<td>6.5712e-003</td>
</tr>
</tbody>
</table>

| order | 1.9336 | 2.0179 | 2.0875 | 2.0274 |

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\lambda_5$</th>
<th>$\lambda_6$</th>
<th>$\lambda_7$</th>
<th>$\lambda_8$</th>
<th>$\lambda_9$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>1.1403e+000</td>
<td>1.4781e+000</td>
<td>1.2502e+000</td>
<td>2.9893e+000</td>
<td>4.7633e+000</td>
</tr>
<tr>
<td>16</td>
<td>2.8814e-001</td>
<td>3.9076e-001</td>
<td>2.9221e-001</td>
<td>7.8135e-001</td>
<td>1.2320e+000</td>
</tr>
<tr>
<td>32</td>
<td>7.2037e-002</td>
<td>9.9434e-002</td>
<td>7.1655e-002</td>
<td>1.9735e-001</td>
<td>3.1058e-001</td>
</tr>
<tr>
<td>64</td>
<td>1.7814e-002</td>
<td>2.5291e-002</td>
<td>1.7768e-002</td>
<td>4.9209e-002</td>
<td>7.7667e-002</td>
</tr>
</tbody>
</table>

| order | 2.0001 | 1.9581 | 2.0438 | 1.9759 | 1.9804 |

Table 3.12: Errors in the eigenvalues determined by the finite difference method applied to the Robin problem with variable coefficient.
CHAPTER 4

OPTIMIZATION PROBLEM IN $\mathbb{R}^N$

4.1 Numerical Methods

In this section, a new iterative method is proposed to find the optimal density configuration for the extremal eigenvalue problems for composite membranes based on previous research work \cite{28}. Unlike the classical level set method \cite{48} based on shape derivatives, this method not only handles the topology changes but also converges efficiently. This section is organized as follows. In section 4.1.1, a fully sorting algorithm based on Rayleigh principle of eigenvalues \cite{28} will be introduced. However, this algorithm encounters difficulty for degenerate eigenvalues. Section 4.1.2 describes a linear programming algorithm to handle the maximization for the ratio of adjacent eigenvalues. Finally, Section 4.1.3 presents a partial sorting algorithm which is designed to handle the degeneracy at a multiple eigenvalue. The efficiency of all these techniques is demonstrated by application to many elliptic eigenvalue problems for composite membranes with different boundary conditions and the numerical results are given in Section 4.2.
4.1.1 Fully Sorting

The shape optimization problem on a fixed domain $\Omega \in \mathbb{R}^2$ with the Dirichlet boundary requires the solution to

$$
-\Delta u = \lambda \rho(x) u, \quad x \in \Omega,
$$

$$
u = 0, \quad x \in \partial \Omega,
$$

where the density $\rho(x)$ is a piecewise constant function

$$
\rho(x) = \begin{cases} 
\rho_1 & \text{for } x \in D \\
\rho_2 & \text{for } x \notin D,
\end{cases}
$$

where $D \subset \Omega$ is a bounded subset inside $\Omega$ and $0 < \rho_1 \leq \rho_2 < \infty$ are constants. The goal is to find

$$
\min_{\rho(x)} \lambda_k \text{ or } \max_{\rho(x)} \lambda_k \text{ or } \frac{\max \lambda_{k+1}}{\lambda_k},
$$

subject to the assumption of fixed weight

$$
\int_{\Omega} \rho(x) dx = K,
$$

where $K$ is a prescribed constant.

The main tool in this endeavor is Rayleigh’s Principle (see Section 2.2)

$$
\lambda_k = \min_{u \in H_0^1(\Omega)} \frac{\int_{\Omega} |\nabla u|^2 dx}{\int_{\Omega} \rho u^2 dx}.
$$

$$
u \perp \text{span}(u_1, \ldots, u_{k-1})
$$

The minimum is attained when $u$ is the associated eigenfunction of $\lambda_k$. The gradient descend approach relies on the computation of the gradient of $\lambda$:

$$
\delta \lambda = -\frac{\left(\int_{\Omega} |\nabla u|^2 dx\right) \left(\int_{\Omega} \delta \rho \cdot u^2 dx\right)}{\left(\int_{\Omega} \rho u^2 dx\right)^2} = -\frac{\lambda \int_{\Omega} \delta \rho \cdot u^2 dx}{\int_{\Omega} \rho u^2 dx}.
$$
By setting
\[ \delta \rho = au^2, \ a > 0, \] (4.7)
and substituting into equation (4.6),
\[ \delta \lambda = -\frac{\lambda a \int_{\Omega} u^4 \, dx}{\int_{\Omega} \rho u^2 \, dx} < 0, \] (4.8)
which guarantees (4.7) is a descent direction. This descent direction implies that the eigenvalue \( \lambda \) decreases as the density function \( \rho(x) \) increases quadratically in \( u \). However, this approach cannot allow piecewise constant distributions of the density function. Instead an iterative fully sorting algorithm can be used so that the constraint on the density function is always satisfied.

The minimization problem for the first eigenvalue is a good play to start a description of the algorithm. The task is to find

\[ \min_{\rho(x)} \lambda_1 = \min_{\rho(x)} \min_{u \in H^1_0(\Omega)} \frac{\int_{\Omega} |\nabla u|^2 \, dx}{\int_{\Omega} \rho u^2 \, dx}, \] (4.9)
subject to constraints (4.2) and (4.4). Assume the eigenfunctions are normalized by \( \int_{\Omega} |\nabla u|^2 \, dx = 1 \). At iteration step \( i \), there is a guess for the configuration density function \( \rho^i \). Use the forward problem solver as discussed in Chapter 3 to find the corresponding eigenvalue \( \lambda_1(\rho^i) \) and eigenfunction \( u_1(\rho^i) \). For simplicity, denote them the eigenpair \( (\lambda_{1,i}, u_{1,i}) \). Thus,
\[ \lambda_{1,i} = \frac{\int_{\Omega} |\nabla u_{1,i}|^2 \, dx}{\int_{\Omega} \rho^i u_{1,i}^2 \, dx}. \] (4.10)

Suppose \( \rho^{i+1} \) is a new guess, such that
\[ \int_{\Omega} \rho^{i+1} u_{1,i}^2 \, dx \geq \int_{\Omega} \rho^i u_{1,i}^2 \, dx. \] (4.11)
Then, a new estimate for $\lambda_{1,i+1}$ will be smaller since

$$\lambda_{1,i+1} = \min_{u \in H^1_0(\Omega)} \frac{\int_{\Omega} |\nabla u| dx}{\int_{\Omega} \rho^{i+1} u^2 dx} = \frac{\int_{\Omega} |\nabla u_{1,i+1}| dx}{\int_{\Omega} \rho^{i+1} u_{1,i+1}^2 dx} \leq \frac{\int_{\Omega} |\nabla u_{1,i}| dx}{\int_{\Omega} \rho^i u_{1,i}^2 dx} = \lambda_{1,i}. \quad (4.12)$$

Therefore, the monotone decreasing sequence $\{\lambda_{1,i}\}$ determined by (4.12) must converge since it has a lower bound.

The success of the procedure depends on (4.11) and there are two ways to satisfy this condition depending on whether the finite element method or the finite difference method is used. The goal is to find a density function $\rho(x)$ so that it can maximize an integral of the form

$$\int_{\Omega} \rho u^2 dx. \quad (4.13)$$

Assume $N$ is the total number of points and $d_j$ is the the density function evaluated at each grid point $P_j$, that is, $d_j = \rho(P_j)$.

For the finite element method, a set of basis functions is available which are defined at each grid point, $\{\Phi_j\}_{j=1}^N$. Representing the maximizer as

$$\rho = \sum_{j=1}^N d_j \Phi_j, \quad (4.14)$$

the integral becomes

$$\int_{\Omega} \rho u^2 dx = \int_{\Omega} \sum_{j=1}^N d_j \Phi_j u^2 dx = \sum_{j=1}^N d_j \int_{\Omega} \Phi_j u^2 dx = \sum_{j=1}^N d_j \psi_j, \quad (4.15)$$

where

$$\psi_j = \int_{\Omega} \Phi_j u^2 dx. \quad (4.16)$$
For the finite difference method, the midpoint rule is used to define the area of a point (see Figure 4.1), say \( A_j = \text{area}(P_j) \). Then integral (4.13) becomes

\[
\int_{\Omega} \rho u_{1,i}^2 dx = \sum_{j=1}^{N} d_j (u_{1,i}^j)^2 A_j, \tag{4.17}
\]

where \( u_{1,i}^j \) is the eigenfunction \( u_{1,i} \) evaluated at point \( P_j \). Denoting

\[
\psi_j = (u_{1,i}^j)^2 A_j, \tag{4.18}
\]

(4.17) becomes

\[
\sum_{j=1}^{N} d_j \psi_j, \tag{4.19}
\]

which is the same as (4.15). The definition of area using midpoint rule at a grid point is illustrated in Figure 4.1. Readers are referred to Figure 7.4 for the definition of area at a point in a triangular mesh.

![Figure 4.1: Area definition using midpoint rule at a grid point in a rectangular mesh.](image)
Similarly, a discrete approximation to the fixed weight constraint (4.4) is

\[ \sum_{j=1}^{N} d_j \xi_j = K, \quad (4.20) \]

where

\[ \xi_j = \int_\Omega \Phi_j dx, \quad \text{for the finite element method}, \]

\[ \xi_j = A_j, \quad \text{for the finite difference method}. \quad (4.21) \]

Step (4.11) can now be stated as

\[ \max_{d=(d_1, \ldots, d_N)} \sum_{j=1}^{N} d_j \psi_j, \quad (4.22) \]

subject to constraints (4.20) and \( d_j \in \{\rho_1, \rho_2\} \), with \( \psi_j \) defined in (4.16) and (4.18) depending on the method used. First sort the discrete values \( \psi_j \) in ascending order. By reindexing the function \( \psi \) if necessary, we may assume

\[ 0 \leq \psi_1 \leq \psi_2 \cdots \leq \psi_N. \quad (4.23) \]

Then it becomes clear that the combination \( \sum_{j=1}^{N} d_j \psi_j \) with

\[ \rho_1 = d_1 \leq d_2 \cdots \leq d_N = \rho_2 \quad (4.24) \]

will give the largest value among all choices of \( d = (d_1, \ldots, d_N) \). (See the proof of Theorem 4.1.3.) Noting that the density function values \( d_j \) is binary, (4.20) can be written as

\[ \rho_1 \sum_{\{j: d_j = \rho_1\}} \xi_j + \rho_2 \sum_{\{j: d_j = \rho_2\}} \xi_j = \rho_1 |D| + \rho_2 (|\Omega| - |D|) = K, \quad (4.25) \]
where

\[ |D| = \begin{cases} 
\sum_{j \in D} \int_{D} \Phi_j dx, & \text{for the finite element method,} \\
\sum_{j \in D} A_j = \text{set area}, & \text{for the finite difference method.} 
\end{cases} \]  

(4.26)

The constraint (4.25) leads directly to the statement

\[ |D| = \frac{\rho_2 |\Omega| - K}{\rho_2 - \rho_1}. \]  

(4.27)

This is the criterion for determining the threshold of the density function.

**Remark 4.1.1** In the numerical computation, interpolation of the point values gives the cell unit values, for example, on a triangular mesh, values from the vertexes are used in the interpolation to the centroid in each triangle. In particular, a uniform triangular mesh like Figure 4.2 is used to reduce possible effects from meshes. In a rectangular uniform mesh, interpolate the values from the grid points to the center of each subsquare. A summary of the new quantities is:

\[
N : \quad \text{total number of cell units,} \\
d_j : \quad \text{density value of cell unit } j, \\
\xi_j : \quad \text{area of cell unit } j, \\
\psi_j : \quad \left(u_{1,i}^j\right)^2 \xi_j, \\
|D| : \quad \text{area of the set with density } \rho_1. 
\]  

(4.28)

Finally, the determination of the threshold of the density function follows from (4.27). Assume the mesh is uniform. The cell unit is either a triangle (triangular mesh) or
Figure 4.2: An example of a uniform triangular mesh with the same area for each triangle.

a square (rectangular mesh). The $\xi_j$’s are the same for every cell unit $\xi_j = |\Omega|/N$. Thus, the threshold for distinguishing $\rho_1$ and $\rho_2$ will be at index

$$j^* = \frac{|D|}{\xi_j} = \frac{(\rho_2|\Omega| - K) / (\rho_2 - \rho_1)}{|\Omega|/N}, \quad (4.29)$$

that is, (4.24) is in fact

$$\rho_1 = d_1 = \cdots d_{j^*} < d_{j^*+1} = \cdots = d_N = \rho_2. \quad (4.30)$$

Since the $\xi_j$’s are the same everywhere, only the squared values $(u_{1,i}^2)$ are used for sorting $\psi_j$.

**Remark 4.1.2** $j^*$ must be an integer. Usually during the numerical implementation, $j^*$ is rounded to satisfy the fixed weight constraint within a prescribed tolerance. To illustrate (4.29) and (4.30), take the unit square as an example, $|\Omega| = 1$. Let $\rho_1 = 1$, $\rho_2 = 2$, and $K = 1.5$. The criterion (4.27) determines the area of the optimal
set $|D| = 0.5$. If there are $N = 100$ units, the area of each unit is $\xi_j = 0.01$. From (4.29) and (4.30), $j^* = 50$ and the density values are distributed as

$$
\begin{align*}
  d_{1-50} &= 1, \\
  d_{51-100} &= 2.
\end{align*}
$$

In terms of the geographic distribution on the unit square, half of the units with smaller $\psi$ values are assigned the smaller density value $\rho_1 = 1$, and half of the units with larger $\psi$ values are assigned the larger density value $\rho_2 = 2$.

Analogous argument follows for other simple eigenvalue minimization problems. A summary of the fully sorting method is described in Algorithm 1.

**Algorithm 1 Fully Sorting Algorithm for Minimization**

- initial guess for $\rho(x)$
- do while not optimal
  1. solve the elliptic eigenvalue problem (4.1) by any forward eigenvalue solver discussed in Chapter 3
  2. sorting $\psi_j$ as in (4.28) in ascending order and compute threshold index $j^*$ as defined in (4.29)
  3. update $\rho(x)$ by the process (4.30)

The maximization problem becomes much more complicated since it requires the
determination of the maximum of a minimum instead of the minimum of a minimum.

The iteration procedure to determine

$$\max_{\rho(x)} \lambda_1 = \max_{\rho(x)} \min_{u \in H_0^1(\Omega)} \frac{\int_{\Omega} \nabla u^2 dx}{\int_{\Omega} \rho u^2 dx},$$

seeks a density function $\rho^{i+1}$, such that

$$\int_{\Omega} \rho^{i+1} u_{1,i}^2 dx \leq \int_{\Omega} \rho^i u_{1,i}^2 dx.$$  \hspace{1cm} (4.33)

In this way,

$$\lambda_{1,i+1} = \frac{\int_{\Omega} |\nabla u_{1,i+1}|^2 dx}{\int_{\Omega} \rho^{i+1} u_{1,i+1}^2 dx} \leq \frac{\int_{\Omega} |\nabla u_{1,i}|^2 dx}{\int_{\Omega} \rho^{i+1} u_{1,i}^2 dx} \geq \frac{\int_{\Omega} |\nabla u_{1,i}|^2 dx}{\int_{\Omega} \rho^i u_{1,i}^2 dx} = \lambda_{1,i}. \hspace{1cm} (4.34)$$

The strategy to guarantee a monotone increasing sequence is to add an acceptance-rejection step. After updating the density function according to (4.33), the forward eigenvalue problem is solved to check if this new configuration actually increases the eigenvalue. If the eigenvalue is increasing, the new configuration of the density function will be accepted, otherwise, another method will be used to update the density function, the so-called Partial Swapping Method, which will be introduced in Section 4.1.3.

In similar line of reasoning adapted to the minimization problem allows one way to achieve (4.33). In this case, the approach is to find

$$\min_{d=(d_1, \ldots, d_N)} \sum_{j=1}^{N} d_j \psi_j.$$  \hspace{1cm} (4.35)

If necessary, $\psi_j$ may be sorted and reindexed to ensure $0 \leq \psi_1 \leq \psi_2 \cdots \leq \psi_N$. Then use the following theorem, which is developed by Wayne [65], allows the construction of the next guess for density function by exploiting (4.35).
**Theorem 4.1.3** Let $a_1 \leq a_2 \leq \ldots \leq a_n$ and $b_1 \leq b_2 \leq \ldots \leq b_n$ be ordered sequences of real numbers. The inequality $a_n b_1 + \ldots + a_1 b_n \leq a_{\sigma(1)} b_1 + a_{\sigma(2)} b_2 + \ldots + a_{\sigma(n)} b_n \leq a_1 b_1 + a_2 b_2 + \ldots + a_n b_n$ holds for every choice of permutation $a_{\sigma(1)}, \ldots, a_{\sigma(n)}$ of $a_1, \ldots, a_n$.

**Proof.** The lower bound follows by applying the upper bound to $-a_n \leq \cdots \leq -a_1$. Therefore, it suffices to prove the upper bound. Since there are only finitely many permutations, there exists at least one for which $a_{\sigma(1)} b_1 + \cdots + a_{\sigma(n)} b_n$ is maximal. If there are several permutations with this property, let $\sigma$ denote the one with the highest number of fixed points.

The proof proceeds by contradiction to establish that $\sigma$ has to be the identity. Assume that $\sigma$ is not the identity. Then there exists a $j$ in $\{1, \cdots, n-1\}$ such that $\sigma(j) \neq j$ and $\sigma(i) = i$ for all $i$ in $\{1, \cdots, j-1\}$. Hence $\sigma(j) > j$ and there exists $k$ in $\{j+1, \cdots, n\}$ with $\sigma(k) = j$. Now

\[ j < k \Rightarrow b_j \leq b_k \quad \text{and} \quad j = \sigma(k) < \sigma(j) \Rightarrow a_j \leq a_{\sigma(j)}. \]

Therefore,

\[ 0 \leq (a_{\sigma(j)} - a_j) (b_k - b_j). \]

Expanding this product and rearranging gives

\[ a_{\sigma(j)} b_j + a_j b_k \leq a_j b_j + a_{\sigma(j)} b_k, \]

hence the permutation

\[
\tau(i) := \begin{cases} 
i & i \in \{1, \cdots, j\}, \\
\sigma(j) & i = k, \\
\sigma(i) & i \in \{j+1, \cdots, n\} \setminus \{k\}, \end{cases}
\]

62
which arises from $\sigma$ by exchanging the values $\sigma(j)$ and $\sigma(k)$, has at least one additional fixed point compared to $\sigma$, namely at $j$, and also attains the maximum. This contradicts the choice of $\sigma$.

If $a_1 < \cdots < a_n$ and $b_1 < \cdots < b_n$, then there are strict inequalities in the above derivation, hence the maximum can only be attained by the identity, any other permutation $\sigma$ cannot be optimal. $\blacksquare$

The above theorem suggests a strategy to update the density function by placing small density at the locations with large $\phi$ values and vice versa. Adopting the definition of the threshold index $j^*$ in (4.29), the density function can be updated by the choice

$$\rho_2 = d_1 = \cdots d_{N-j^*} > d_{N-j^*+1} = \cdots = d_N = \rho_1.$$  \hspace{1cm} (4.36)

This approach based on sorting can be easily generalized to higher eigenmodes. Unfortunately, the process does not guarantee monotone decreasing. Instead, a different approach, the partial swapping method, will be used. A summary of the fully sorting method for the maximization problem is provided in Algorithm 2.
Algorithm 2 Fully Sorting Algorithm for Maximization

initial guess for $\rho(x)$

solve the elliptic eigenvalue problem (4.1) by any forward eigenvalue solver discussed in Chapter 3

do while not optimal

1. sorting $\psi_j$ as in (4.28) in ascending order and compute threshold index $j^*$ as defined in (4.29)

2. update $\rho(x)$ by the process (4.36)

3. solve the elliptic eigenvalue problem using updated $\rho(x)$

- if the eigenvalue increases, accept $\rho(x)$
- if not, use Partial Swapping Method to generate a new $\rho(x)$

4.1.2 Linear Fractional Programming

The third type of optimization problem is to find

$$ \max_{\rho(x)} \frac{\lambda_{k+1}}{\lambda_k} = \max_{\rho(x)} \frac{\min_{w_1} \int_{\Omega} |\nabla w_1|^2 dx}{\min_{w_2} \int_{\Omega} \rho w_2^2 dx} $$

where

$$ w_1 \in \{ w \in H_0^1(\Omega) : w \perp \text{span}(u_1, \ldots, u_k) \} $$

$$ w_2 \in \{ w \in H_0^1(\Omega) : w \perp \text{span}(u_1, \ldots, u_{k-1}) \} $$
The design of an iterative procedure to find the maximum is based on the expression,

\[
\frac{\lambda_{k+1}}{\lambda_k} = \frac{\int_{\Omega} |\nabla u_{k+1}|^2 \, dx}{\int_{\Omega} |\nabla u_k|^2 \, dx} \cdot \frac{\int_{\Omega} \rho u_{k+1}^2 \, dx}{\int_{\Omega} \rho u_k^2 \, dx},
\]

(4.39)

where the eigenpairs \((\lambda_{k+1}, u_{k+1})\), \((\lambda_k, u_k)\) are the solutions of equation (4.1). Notice that in (4.39) only the second ratio contains the density function \(\rho(x)\). The way to treat this ratio follows the approach developed for the integral of type (4.13). As a consequence, the search for the maximum of \(\lambda_{k+1}/\lambda_k\) becomes a quest to find

\[
\max_{d=(d_1, \ldots, d_N)} \frac{\sum_{j=1}^{N} d_j \psi_j^{(k)}}{\sum_{j=1}^{N} d_j \psi_j^{(k+1)}},
\]

(4.40)

subject to the constraints (4.20) and \(d_j \in \{\rho_1, \rho_2\}\) where \(N, d_j, \) and \(\psi_j\) are defined as in (4.28) and the superscripts on \(\psi_j\) are used to distinguish the corresponding eigenmodes.

Much is known about linear fractional optimization problems of the form (4.40); see [6] for example. In particular, there is a very general algorithm, Dinkelbach’s algorithm, which applies to

\[
\max_{x \in S} \frac{P(x)}{Q(x)},
\]

(4.41)

where \(P(x), Q(x) \geq 0\) are linear functions of \(x\). \(S\) is the feasible set of the optimization problem. Define

\[
F(\lambda) = \max_{x \in S} \{ P(x) - \lambda Q(x) \}, \lambda \in \mathcal{R}.
\]

(4.42)

The Dinkelbach’s algorithm is supported by the following theorem.
Theorem 4.1.4 \ Vector \ x^* \ is \ an \ optimal \ solution \ of \ problem \ (4.41) \ if \ and \ only \ if
\[ F(\lambda^*) = \max_{x \in S} \{P(x) - \lambda^*Q(x)\} = 0 \] (4.43)

where
\[ \lambda^* = \frac{P(x^*)}{Q(x^*)}. \] (4.44)

Proof. If vector \ x^* \ is an optimal solution of (4.41), then
\[ \lambda^* = \frac{P(x^*)}{Q(x^*)} \geq \frac{P(x)}{Q(x)}, \ \forall x \in S. \]
That is,
\[ P(x) - \lambda^*Q(x) \leq 0, \ \forall x \in S. \]

Note that
\[ P(x^*) - \lambda^*Q(x^*) = 0, \]
so
\[ \max_{x \in S} \{P(x) - \lambda^*Q(x)\} = 0. \]

On the other hand, if vector \ x^* \ is an optimal solution of (4.43), then
\[ 0 = P(x^*) - \lambda^*Q(x^*) \geq P(x) - \lambda^*Q(x), \ \forall x \in S. \]
That is,
\[ \lambda^* = \frac{P(x^*)}{Q(x^*)} \geq \frac{P(x)}{Q(x)}, \ \forall x \in S. \]

Thus, \ x^* \ is an optimal solution of (4.41).

The above theorem simply converts the optimization of a linear fractional function to the optimization of a linear function. Algorithm 3 can do this.
Algorithm 3 Dinkelbach’s Algorithm

Initial guess for $x^{(0)} \in S$, calculate $\lambda^{(1)} := \frac{P(x^{(0)})}{Q(x^{(0)})}$, set $m = 1$

do while $F(\lambda^{(m)}) \neq 0$

1. $x^{(m)} := \arg \max_{x \in S} \{ P(x) - \lambda^{(m)} Q(x) \}$

2. $\lambda^{(m+1)} := \frac{P(x^{(m)})}{Q(x^{(m)})}$, set $m = m + 1$

Noting that the step for determining

$$\arg \max_{x \in S} \{ P(x) - \lambda^{(m)} Q(x) \} = \arg \max_{d = (d_1, \ldots, d_N)} \sum_{j=1}^{N} d_j (\psi_j^k - \lambda^{(m)} \psi_j^{k-1})$$

is in fact the optimization problem as discussed in (4.22), except that $\psi_j$ is replaced with $\psi_j^k - \lambda^{(m)} \psi_j^{k-1}$. The sorting procedure (4.23) and updating procedure (4.30) can be applied immediately to obtain the optimal configuration.

Finally, a summary of the method for maximizing the ratio of adjacent eigenvalues is presented in Algorithm 4.
Algorithm 4 Algorithm for Maximization the Ratio of Adjacent Eigenvalues

initial guess for \( \rho(x) \)

solve the elliptic eigenvalue problem (4.1) by any forward eigenvalue solver discussed in Chapter 3

do while not optimal

1. update \( \rho(x) \) by solving (4.40) via Dinkelbach’s Algorithm

2. solve the elliptic eigenvalue problem using updated \( \rho(x) \)
   
   - if the eigenvalue ratio increases, accept \( \rho(x) \)
   
   - if not, use Partial Swapping Method to generate a new \( \rho(x) \)

4.1.3 Partial Swapping

Even if the second ratio in equation (4.39) is increased there is no guarantee that the \( \lambda_{K+1}/\lambda_k \) is increased. In other words, monotonicity is not guaranteed. When a configuration of the density function through fully sorting does not increase the eigenvalue, the partial swapping method will be used. Figure 4.3 illustrates this method.
Figure 4.3: An illustration of the partial swapping method. Left panel shows the fully sorting method: switch the density values in the difference sets $A\setminus B$ (light gray region) and $B\setminus A$ (dark gray region). Right panel shows the partial swapping method: switch the density values in the subsets $C$ (light gray region) and $D$ (dark gray region).

Let set $A$ (within the red circle) be the current configuration of the density function with value $\rho_1$, and let set $B$ (within the blue circle) be the suggested configuration with density value $\rho_1$ which is obtained from fully sorting. The left panel in Figure 4.3 illustrates the fully sorting method. If the suggested configuration increases the target eigenvalue, it is accepted, that is, the density values in the difference sets $A\setminus B$ (light gray region) and $B\setminus A$ (dark gray region) are switched. However, if this configuration fails, choose subsets of $A\setminus B$ and $B\setminus A$, say sets $C$ (light gray region) and $D$ (dark gray region) as labeled in Figure 4.3 (right panel), and switch their density.
values. Subsets $C$ and $D$ are of the same size in order to satisfy the fixed weight assumption (4.4). The size of the subsets is a parameter which will be adjusted by trial and error. In the numerical implementation, the size is halved until a density configuration which increases the target eigenvalue is reached.

The selection of the subsets $C$ and $D$ follows the sorting idea. Take $\max_{\rho(x)} \lambda_1$ for example, at iteration step $i$. If the fully sorting method fails, subset $C$ in $A \setminus B$ of prescribed size is generated according to sorting $\psi_j = (u_{1,i}^j)^2 \xi_j$, which is a constant multiple of the squared eigenfunction values, preferring small values. In contrast to the selection of subset $C$, large squared eigenvalues are preferred for the selection of subset $D$. Finally, switch the density values in $C$ and $D$ instead of the $A \setminus B$ and $B \setminus A$. Figure 4.4 illustrates the selection of the subsets $C$ and $D$.

![Diagram](image)

Figure 4.4: An illustration of the selection of the subsets $C$ and $D$. (cyan regions)
4.1.4 Gradient at Degenerate Eigenvalues

So far the techniques discussed above work perfectly for any simple eigenvalue. When the eigenvalue is degenerate, the eigenfunction is not uniquely determined. The update formula of density distribution needs to be adjusted accordingly. It is possible that several density configurations have the same specific eigenvalue. When this happens, the iterative scheme may switch back and forth between two density configurations. This occurs frequently when the eigenvalue becomes degenerate during the iteration process. Thus this section is devoted to the discussion on the update strategy of density distribution for a degenerate eigenvalue. The generalized gradient is considered as the classical derivative does not exist in this case. In the work of S. Cox [12], the strategy for computing the generalized gradient of the extreme eigenvalues has been explained and applied to an elliptic operator. Roughly speaking, for a “nice” operator $A(\rho)$, let $co$ be the convex hull and $DA(\rho_0)$ be the derivative of $A$ at $\rho_0$, we assume a repeating eigenvalue has multiplicity $m$:

$$\lambda_{k-1}(\rho_0) < \lambda_k(\rho_0) = \cdots = \lambda_{k+m-1}(\rho_0) < \lambda_{k+m}(\rho_0), \ m > 1. \quad (4.45)$$

Then

$$\partial \lambda_k(\rho_0) = \partial \lambda_{k+m-1}(\rho_0) = \left\{co \left(\langle DA(\rho_0), \cdot \rangle u, u \rangle_H : u \in \varepsilon^1_k(\rho_0)\right) \right\}$$,

(4.46)

where $\langle \cdot, \cdot \rangle$ is the inner product on a Hilbert space $H$, $\varepsilon^1_k(\rho)$ is the intersection of the span of the $k$th eigenfunction with the unit sphere.

Applying the idea in (4.36), the choice of the gradient direction at a multiple eigenvalue is

$$co \left(u^2_j\right), \ j = k, \cdots k + m - 1,$$

(4.47)
where \( u_j \) is the \( j \)th eigenfunction. In applications, instead of using a threshold to determine how close the adjacent eigenvalues are, the convex hull is always used as the gradient direction from the beginning of the process. The most common eigenvalues are of multiplicity 2. For example, \( \lambda_k(\rho_0) = \lambda_{k+1}(\rho_0) \), then the linear combination

\[
\psi = \alpha u_k^2 + (1 - \alpha)u_{k+1}^2, \quad 0 < \alpha < 1,
\]

is used as the reference function in the process (4.22), (4.35), and (4.40). Here \( \alpha \) is parameter to be adjusted and \( \alpha = \frac{1}{2} \) is used in most computations.

### 4.2 Numerical Results

In this section, results of the numerical algorithm described in Section 4.1 will be presented in three parts. First, \( \max_{\rho} \lambda_k \) with different boundary conditions will be given. The results of \( \min_{\rho} \lambda_k \) problems have appeared in previous research work on the fully sorting method [28]. Second, the role of the Robin type boundary parameter in the optimization results is investigated. The same initial guess is used for different \( \beta \) values. Starting with the Dirichlet boundary condition, the weighting parameter \( \beta \) is gradually decreased until the Neumann Boundary condition is reached. The evolution of the optimal result under this process proves interesting. Finally, the results of \( \max_{\rho} \lambda_{k+1}/\lambda_k \) with the Dirichlet boundary condition are presented.
4.2.1 \( \max_\rho \lambda_k \)

**Dirichlet Boundary Condition** For convenience, the governing equation is restated:

\[
-\Delta u = \lambda \rho(x) u, \quad x \in \Omega, \quad u = 0, \quad x \in \partial \Omega,
\]

and \( \max_\rho \lambda_k^D \) will denote to indicate the Dirichlet boundary condition. The domain is set as \( \Omega = [0, 1] \times [0, 1] \), \( \rho_1 = 1 \) (black), \( \rho_2 = 2 \) (white), and \( K = 3/2 \) is fixed for all the numerical results generated in Sections 4.2.1 and 4.2.2. Thus, the measure of the optimal set is 1/2, i.e., half of the domain has density value \( \rho_1 = 1 \), and the other half has density value \( \rho_2 = 2 \). The same stopping criterion is used for all the simulations. That is, when \( L^2 \) norm of the change between current and previous configuration of the density is less than \( 10^{-10} \). The adjacent eigenvalues is also shown at each iteration step. The iteration step using the partial swapping method is overlayed by a “+” and a filled circle is marked if the generalized gradient (4.48) is applied at degeneracy.

1. \( \max_\rho \lambda_1^D = 18.3951 \)
Figure 4.5: Results at selected iteration steps; darker shading shows region of \( \rho_1 \), and lighter shading shows \( \rho_2 \). \( \max_{\rho} \lambda_1^D = 18.3951 \).

Figure 4.5 shows the results for \( \max_{\rho} \lambda_1 \). The calculations start with an initial guess of two identical circles containing density value \( \rho_2 \), as shown for \( \lambda_1^{(0)} \). Subsequent results for iterations 1 (\( \lambda_1^{(1)} \)), 2 (\( \lambda_1^{(2)} \)), 11 (\( \lambda_1^{(11)} \)) indicate the approach to the maximum. The "optimal" result (\( \lambda_1^{(11)} \)) shows that the places with larger density value \( \rho_2 \) are attached to the boundary. This result is consistent with the theory of Cox-McLaughlin (Theorem 2.3.8). It takes 12 steps to converge. The second row in Figure 4.5 plots the changes in \( \lambda_1 \) and \( \lambda_2 \) (\( \lambda_1 < \lambda_2 \)), which are the
eigenvalues to equation (4.49) under the configuration of the density function at each step. Notice that four decimal places are shown for each iteration. The algorithm starts with an initial mesh of the maximum edge length 1, and it is refined seven times to do the forward and optimization computations for each example. The resulting mesh has the maximum edge length $1/2^7$. Based on the forward cases tested in Chapter 3, the error is within $O(10^{-5})$ up to the first nine eigenvalues. However, the resolution should be further studied for forward problems with complicated interfaces. An example of error estimation in 1D is shown in [56], and [43] shows some numerical simulations with complicated interfaces in 2D. The error gets bigger for the larger eigenvalues.

2. $\max_\rho \lambda_2^D = 42.6309$
Figure 4.6: Results at selected iteration steps; darker shading shows region of 
ρ₁, and lighter shading shows ρ₂. maxₚ λ₂ᵩ = 42.6309.

Figure 4.6 shows the results for maxₚ λ₂. The calculations start with the same
initial guess of two identical circles containing density value ρ₂, shown for λ₂⁽⁰⁾,
and the subsequent results for iterations 1 (λ₂⁽¹⁾), 2 (λ₂⁽²⁾), 15 (λ₂⁽¹⁵⁾) show conver-
gence to the maximum configuration. The "optimal" result (λ₂⁽¹⁵⁾) shows that
the places with smaller density value ρ₁ look like a square washer. It takes 16
steps to converge. The second row in Figure 4.6 plots the changes in eigenvalues
λ₁₋₄ at each iteration. There is a degeneracy in λ₂; the generalized gradient
idea applies here. A linear combination $\psi = \frac{1}{2}(u_2^2 + u_3^2)$ is used in the sorting process at each step, where $u_2$ and $u_3$ are the corresponding eigenfunctions.

3. $\max_{\rho} \lambda_3^D = 47.2711$

Figure 4.7: Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_{\rho} \lambda_3^D = 47.2711$. 

Figure 4.7 shows the results for $\max_{\rho} \lambda_3$. The calculations start with the same initial guess of two identical circles, shown for $\lambda_3^{(0)}$, and subsequent results for
iterations 1 \( (\lambda_3^{(1)}) \), 2 \( (\lambda_3^{(2)}) \), 12 \( (\lambda_3^{(12)}) \) show the convergence to the maximum. The "optimal" result \( (\lambda_3^{(12)}) \) shows that the places with smaller density value \( \rho_1 \) look like two triangles along the diagonal. It takes 13 steps to converge. The second row in Figure 4.7 plots the changes in eigenvalues \( \lambda_{2-4} \). 

4. \( \max_{\rho} \lambda_4^D = 70.7599 \)

![Graph showing eigenvalues and iteration steps](image)

Figure 4.8: Results at selected iteration steps; darker shading shows region of \( \rho_1 \), and lighter shading shows \( \rho_2 \). \( \max_{\rho} \lambda_4^D = 70.7599 \).
Figure 4.8 shows the results for $\max_\rho \lambda_4$. The calculations start start with the initial guess of one circle centered with density value $\rho_1$, shown for $\lambda_4^{(0)}$, and the subsequent results for iterations 1 ($\lambda_4^{(1)}$), 2 ($\lambda_4^{(2)}$), 13 ($\lambda_4^{(13)}$) show the convergence to an optimal result. The "optimal" result ($\lambda_4^{(13)}$) shows that the places with smaller density value $\rho_1$ look like a flower. It takes 14 steps to converge. The second row in Figure 4.8 plots the changes in eigenvalues $\lambda_{3-6}$. There is a degeneracy in $\lambda_4$, so a linear combination $\psi = 0.1u_4^2 + 0.7u_5^2 + 0.2u_6^2$ is used in the sorting process at each step, where $u_{4-6}$ are the corresponding eigenfunctions.

**Neumann Boundary Condition** The governing equation is

$$-\Delta u = \lambda \rho(x) u, \quad x \in \Omega,$$

$$\frac{\partial u}{\partial n} = 0, \quad x \in \partial \Omega. \quad (4.50)$$

Similarly, the notation $\max_\rho \lambda_k^N$ indicates the Neumann boundary condition. Notice that we only label the positive eigenvalues. For Neumann boundary problems, $\lambda_1 = 0$ is an eigenvalue associated with a constant eigenfunction. It is the positive eigenvalues that are of interest. The optimal results for the $k$th eigenmode with Neumann boundary are then compared to the $(k + 1)$th eigenmode with the Dirichlet or Robin boundary conditions.

1. $\max_\rho \lambda_2^N = 9.1975$
Figure 4.9: Results at selected iteration steps; darker shading shows region of \( \rho_1 \), and lighter shading shows \( \rho_2 \). \( \max_\rho \lambda_2^N = 9.1975 \).

Figure 4.9 shows the results for \( \max_\rho \lambda_2 \). The calculations start with an initial guess of two identical circles, as shown for \( \lambda_2^{(0)} \), and the subsequent results for iterations 1 (\( \lambda_2^{(1)} \)), 2 (\( \lambda_2^{(2)} \)), 5 (\( \lambda_2^{(5)} \)) show convergence to the optimal solution. The "optimal" result (\( \lambda_2^{(5)} \)) shows that the places with smaller density value \( \rho_1 \) are fan-like and attached to the diagonal corners. It takes 6 steps to converge. The second row in Figure 4.9 plots the changes in eigenvalues \( \lambda_{1-3} \), which are
the eigenvalues to equation (4.50) under the configuration of density function at each step.

2. \( \max_\rho \lambda_3^N = 18.3951 \)

Figure 4.10: Results at selected iteration steps; darker shading shows region of \( \rho_1 \), and lighter shading shows \( \rho_2 \). \( \max_\rho \lambda_3^N = 18.3951 \).

Figure 4.10 shows the results for \( \max_\rho \lambda_3 \). The calculations start with an initial guess of two identical circles, as shown for \( \lambda_3^{(0)} \), and the subsequent results for
iterations 1 ($\lambda_3^{(1)}$), 2 ($\lambda_3^{(2)}$), 7 ($\lambda_3^{(7)}$) show convergence to the optimal solution. The "optimal" result ($\lambda_3^{(7)}$) shows that the places with larger density value $\rho_2$ look like a cross. It takes 8 steps to converge. The second row in Figure 4.10 plots the changes in eigenvalues $\lambda_2-4$.

3. max$_\rho \lambda_4^N = 29.8931$

Figure 4.11: Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. max$_\rho \lambda_4^N = 29.8931$. 
Figure 4.11 shows the results for \( \max_p \lambda_4 \). The calculations start with an initial guess of nine identical circles containing density value \( \rho_2 \), as shown for \( \lambda_4^{(0)} \), and the subsequent results for iterations 1 (\( \lambda_4^{(1)} \)), 2 (\( \lambda_4^{(2)} \)), 10 (\( \lambda_4^{(10)} \)) show convergence to the optimal solution. The "optimal" result (\( \lambda_4^{(10)} \)) shows that the places with larger density value \( \rho_2 \) look like four squares along the diagonals. It takes 11 steps to converge. The second row in Figure 4.11 plots the changes in eigenvalues \( \lambda_{3-6} \). There is a degeneracy in \( \lambda_4 \), so a linear combination \( \psi = \frac{1}{2}(u_4^2 + u_5^2) \) is used in the sorting process at each step, where \( u_4 \) and \( u_5 \) are the corresponding eigenfunctions.

**Robin Boundary Condition**  The governing equation is

\[
-\Delta u = \lambda \rho(x) u, \quad x \in \Omega, \\
\frac{\partial u}{\partial n} + \beta u = 0, \quad x \in \partial \Omega.
\] (4.51)

Similarly, the notation \( \max_p \lambda_k^R \) indicates the Robin boundary condition. Various choices of \( \beta \) are made.

1. \( \max_p \lambda_1^R = 2.3839, \ \beta = 1 \)
Figure 4.12: Results at selected iteration steps; darker shading shows region of \( \rho_1 \), and lighter shading shows \( \rho_2 \). \( \max_{\rho} \lambda^R_1 = 2.3839 \), \( \beta = 1 \).

Figure 4.12 shows the results for \( \max_{\rho} \lambda_1 \) when \( \beta = 1 \). The calculations start with an initial guess of four identical circles containing density value \( \rho_2 \), as shown for \( \lambda_1^{(0)} \), and the subsequent results for iterations 1 (\( \lambda_1^{(1)} \)), 2 (\( \lambda_1^{(2)} \)), 6 (\( \lambda_1^{(6)} \)) show convergence. The "optimal" result (\( \lambda_1^{(6)} \)) is similar to the result for the Dirichlet boundary \( \max_{\rho} \lambda_1^D \). The places with larger density value \( \rho_2 \) are attached to the boundary. It takes 7 steps to converge. The second row in

84
Figure 4.12 plots the changes in eigenvalues \( \lambda_{1-2} \), which are the eigenvalues to equation (4.51) with parameter \( \beta = 1 \) under the configuration of density function at each step.

2. \( \max_\rho \lambda_3^R = 31.3343, \ \beta = 10 \)

![Figure 4.12: Results at selected iteration steps; darker shading shows region of \( \rho_1 \), and lighter shading shows \( \rho_2 \). \( \max_\rho \lambda_3^R = 31.3343, \ \beta = 10 \)](image)

Figure 4.13 shows the results for \( \max_\rho \lambda_3 \) when \( \beta = 10 \). The calculation starts
with a slightly different initial guess of four identical circles containing density value $\rho_2$, as shown for $\lambda_3^{(0)}$, and the subsequent results for iterations 1 ($\lambda_3^{(1)}$), 2 ($\lambda_3^{(2)}$), 14 ($\lambda_3^{(14)}$) show convergence. The "optimal" result ($\lambda_3^{(14)}$) is also similar to the result for the Dirichlet boundary $\max_\rho \lambda_3^D$. The places with smaller density value $\rho_1$ look like two triangles along the diagonal. It takes 15 steps to converge. The second row in Figure 4.13 plots the changes in eigenvalues $\lambda_{2-4}$, which are the eigenvalues to equation (4.51) with parameter $\beta = 10$.

3. $\max_\rho \lambda_4^R = 24.5825$, $\beta = 1$
Figure 4.14: Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_\rho \lambda_4^R = 24.5825$, $\beta = 1$.

Figure 4.14 shows the results for $\max_\rho \lambda_4$ when $\beta = 1$. The calculations start with an initial guess of four identical circles containing density value $\rho_2$, as shown for $\lambda_4^{(0)}$, and the subsequent results for iterations 1 ($\lambda_4^{(1)}$), 2 ($\lambda_4^{(2)}$), 7 ($\lambda_4^{(7)}$) show convergence. The optimal result ($\lambda_4^{(7)}$) is similar to the result for the Neumann boundary $\max_\rho \lambda_3^N$. The places with larger density value $\rho_2$ look like a cross. It takes 8 steps to converge. The second row in Figure 4.14 plots
the changes in eigenvalues $\lambda_{3-5}$, which are the eigenvalues to equation (4.51) with parameter $\beta = 1$.

4.2.2 Investigating Robin Boundary Parameter $\beta$

Due to the non-degeneracy at eigenmode $\lambda_3$, we now investigate the role of the Robin boundary parameter $\beta$ in the maximization problem $\max_{\rho} \lambda_{3}^{R}$. As $\beta \to \infty$, the Robin boundary condition asymptotes to the Dirichlet boundary condition, shown as the first graph in Figure 4.15 for comparison purpose. As $\beta \to 0$, the Robin boundary condition becomes the Neumann boundary condition, shown as the last graph in the sequence.
Figure 4.15: Investigating Robin parameter $\beta$; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$.

The initial guess of two identical circles with density value $\rho_2$ is used for all the computations. (Note that result for $\max_\rho \lambda_2^N$ is shown here.) Figure 4.14 shows the optimal results for $\beta = 10, 4, 3, 1, 0.5, 0.01$, and the two extreme cases (Dirichlet and Neumann boundary problems). There is a gradual change as the two triangle shaped regions with density $\rho_1$ are pushed to the diagonal corners and then morph into two fan-like regions.
4.2.3 \( \max_\rho \lambda_{k+1}/\lambda_k \)

For the maximization of the ratio of adjacent eigenvalues, only the Dirichlet Boundary problems will be considered.

1. \( \max_\rho \lambda_2/\lambda_1 = 2.5959 \)

Figure 4.16: Results at selected iteration steps; darker shading shows region of \( \rho_1 \), and lighter shading shows \( \rho_2 \). \( \max_\rho \lambda_2/\lambda_1 = 2.5959 \).
Figure 4.16 shows the results for \( \max_\rho \lambda_2 / \lambda_1 \). The calculations start with an initial guess of one circle containing density value \( \rho_2 \), as shown for \((\lambda_2 / \lambda_1)^{(0)}\), and the subsequent results for iterations 1 \((\lambda_2 / \lambda_1)^{(1)}\), 2 \((\lambda_2 / \lambda_1)^{(2)}\), 3 \((\lambda_2 / \lambda_1)^{(3)}\) show convergence. It takes 4 steps to converge. The second row in Figure 4.16 plots the changes in eigenvalues \( \lambda_1-2 \).

2. \( \max_\rho \lambda_3 / \lambda_2 = 2.1439 \)

Figure 4.17: Results at selected iteration steps; darker shading shows region of \( \rho_1 \), and lighter shading shows \( \rho_2 \). \( \max_\rho \lambda_3 / \lambda_2 = 2.1439 \).
Figure 4.17 shows the results for \( \max_{\rho} \lambda_3/\lambda_2 \). The calculations start with an initial guess of two identical circles containing density value \( \rho_2 \), as shown for \((\lambda_3/\lambda_2)^{(0)}\), and the subsequent results for iterations 1 \(((\lambda_3/\lambda_2)^{(1)})\), 2 \(((\lambda_3/\lambda_2)^{(2)})\), 6 \(((\lambda_3/\lambda_2)^{(6)})\) show convergence. It takes 7 steps to converge. The second row in Figure 4.17 plots the changes in eigenvalues \( \lambda_{1-4} \). There is a degeneracy in \( \lambda_3 \), so a linear combination \( \psi = \frac{1}{2}(u_3^2 + u_4^2) \) is used in the sorting process at each step, where \( u_{3-4} \) are the corresponding eigenfunctions. One may wonder why the optimal configuration looks closer to the result of \((\lambda_3/\lambda_2)^{(1)}\) than that of \((\lambda_3/\lambda_2)^{(2)}\). This is due to the partial swapping method. It turns out that the optimal configuration is between the results shown in \((\lambda_3/\lambda_2)^{(1)}\) and \((\lambda_3/\lambda_2)^{(2)}\).

At iteration 2, fully sorting method directly increases the ratio \( \lambda_3/\lambda_2 \). However, as the ratio keeps increasing, it becomes harder for the fully sorting method to directly increase the ratio, thus the partial swapping is used and it fine-tunes the result to be optimal.

3. \( \max_{\rho} \lambda_4/\lambda_3 = 1.6004 \)
Figure 4.18: Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max_{\rho} \frac{\lambda_4}{\lambda_3} = 1.6004$.

Figure 4.18 shows the results for $\max_{\rho} \frac{\lambda_4}{\lambda_3}$. The calculations start with an initial guess of one circle containing density value $\rho_2$, as shown for $(\lambda_4/\lambda_3)^{(0)}$, and the subsequent results for iterations 1 ($(\lambda_4/\lambda_3)^{(1)}$), 29 ($(\lambda_4/\lambda_3)^{(29)}$), 64 ($(\lambda_4/\lambda_3)^{(64)}$) show convergence. It takes 65 steps to converge. The second row in Figure 4.18 plots the changes in eigenvalues $\lambda_2$–$5$. There is a degeneracy in
\( \lambda_4 \), so a linear combination \( \psi = \frac{1}{2} (u_4^2 + u_5^2) \) is used in the sorting process at each step, where \( u_{4-5} \) are the corresponding eigenfunctions.

4. \( \max_\rho \lambda_5/\lambda_4 = 1.6865 \)

Figure 4.19: Results at selected iteration steps; darker shading shows region of \( \rho_1 \), and lighter shading shows \( \rho_2 \). \( \max_\rho \lambda_5/\lambda_4 = 1.6865 \).

Figure 4.19 shows the results for \( \max_\rho \lambda_5/\lambda_4 \). The calculations start with an initial guess of two identical circles containing density value \( \rho_2 \), as shown for
$(\lambda_5/\lambda_4)^{(0)}$, and the subsequent results for iterations 1 ($(\lambda_5/\lambda_4)^{(1)}$), 2 ($(\lambda_5/\lambda_4)^{(2)}$), 13 ($(\lambda_5/\lambda_4)^{(13)}$) show convergence. It takes 14 steps to converge. The second row in Figure 4.19 plots the changes in eigenvalues $\lambda_{3-6}$. There is a degeneracy in $\lambda_4$, so a linear combination $\psi = \frac{1}{2}(u_3^2 + u_4^2)$ is used in the sorting process at each step, where $u_{3-4}$ are the corresponding eigenfunctions.

5. $\max \rho \lambda_6/\lambda_5 = 1.7707$

---

Figure 4.20: Results at selected iteration steps; darker shading shows region of $\rho_1$, and lighter shading shows $\rho_2$. $\max \rho \lambda_6/\lambda_5 = 1.7707$. 

95
Figure 4.20 shows the results for \( \max_\rho \lambda_6/\lambda_5 \). The calculations start with an initial guess of four identical circles containing density value \( \rho_2 \), as shown for \( (\lambda_6/\lambda_5)^{(0)} \), and the subsequent results for iterations 1 \( ((\lambda_6/\lambda_5)^{(1)}) \), 2 \( ((\lambda_6/\lambda_5)^{(2)}) \), 4 \( ((\lambda_6/\lambda_5)^{(4)}) \) show convergence. It takes 5 steps to converge. The second row in Figure 4.20 plots the changes in eigenvalues \( \lambda_{3-7} \). There are degeneracies in \( \lambda_5 \) and \( \lambda_6 \), so linear combinations \( \psi_1 = \frac{1}{2}(u_4^2 + u_5^2) \) and \( \psi_2 = \frac{1}{2}(u_6^2 + u_7^2) \) are used in the sorting process at each step, where \( u_{4-7} \) are the corresponding eigenfunctions.

4.3 Discussion and Conclusion

This work studies the shape optimization of the elliptic eigenvalue problems. A novel numerical approach based on the variational form of the elliptic eigenvalue equation is proposed. It can handle the topological changes automatically without the computation of the shape derivatives. Results for maximizing the \( k \)th eigenvalue with different boundary conditions and maximizing the ratio of adjacent eigenvalues are presented. The numerical results remarkably show the efficiency of this new method in generating the optimal configurations of the density function.

The main strengths of the proposed approach is the fact that it converges much faster than the level set method based algorithms. For most iterative methods, solving the forward elliptic eigenvalue problem is unavoidable at each iteration. Thus it is crucial to reduce the number of iterations in order to speed up the process. This new
approach only takes several iterations to reach the optimal solution while level set method based algorithms usually take hundreds of iterations.

Previous studies mainly focused on the Dirichlet boundary condition and the optimization of the first eigenvalue. By applying the proposed approach to general Robin type boundary conditions, interesting results are produced for the first eigenvalue and higher eigenvalues.

Most algorithms encounter difficulty at the degeneracy of eigenvalues. This work addresses the question of how to deal with degenerate eigenvalues in the numerical implementation. The update formula for density needs to adapt convex combination of multiple eigenfunctions. This overall approach can be further generalized to a wide variety of shape optimization problems.
CHAPTER 5
OPTIMIZATION PROBLEM ON MANIFOLDS

Elliptic eigenvalue problems on manifolds are a natural extension of the previous chapter. For example, in biological implementations, the habitat $\Omega$ of a species can be a surface. The optimal results on manifolds will then be affected by the curvature of the surface. The Laplace operator is generalized to operate on manifolds, and is named the Laplace-Beltrami operator. Like the Laplacian, the Laplace-Beltrami operator is defined as

$$\Delta f = \text{div grad} f.$$  \hfill (5.1)

For a scalar function $f$, the Laplace-Beltrami operator can be written in local coordinates as

$$\Delta f = \frac{1}{\sqrt{|g|}} \partial_i \left( \sqrt{|g|} g^{ij} \partial_j f \right),$$  \hfill (5.2)

where $g^{ij}$ are the elements of the inverse metric tensor $g$. The Riemannian metric $g$ in local coordinates can be written as

$$g = J^T J,$$  \hfill (5.3)

where $J$ is the Jacobian matrix of the coordinate change. In this chapter, the method described in Chapter 4 is extended to solve the eigenvalue minimization problem on
manifolds. The manifolds considered here are restricted to the surfaces which can be presented as a graph of a function.

5.1 1D problems

The problem with the Dirichlet boundary is simply

\[-u_{ss} = \lambda \rho u \quad \text{in} \quad \mathcal{M} \]
\[u = 0 \quad \text{on} \quad \partial \mathcal{M}, \quad (5.4)\]

where \(\mathcal{M}\) is a manifold.

5.1.1 Forward Problem

A simple example helps illustrate the nature of elliptic problems on manifolds.

**Special case** Consider the manifold of a half unit circle

\[x^2 + y^2 = 1, \quad -1 \leq x \leq 1, \quad y \geq 0. \quad (5.5)\]

That is, the eigenvalue problem lies on the manifold

\[\mathcal{M} : \quad y = f(x) = \sqrt{1 - x^2}, \quad -1 \leq x \leq 1. \quad (5.6)\]

The arclength parametrization of the half unit circle is

\[x = \cos s, \quad y = \sin s, \quad (5.7)\]
so,

\[ u_{ss} = (u_x(-\sin s))_x(-\sin s) = (u_x(\sin s))_x(\sin s) \]
\[ = (u_{xx}(\sin s) + u_x(\sin s)_x)(\sin s) \]
\[ = (u_{xx}(\sin s) + u_x y_x)(\sin s) = u_{xx} y^2 + u_x \left(-\frac{x}{\sqrt{1-x^2}}\right)y \]
\[ = u_{xx}(1-x^2) - xu_x. \]

The equation can be written as

\[ -(1-x^2)u_{xx} + xu_x = \lambda pu. \] (5.9)

On the other hand, the definition of the metric (5.3) gives

\[ x = \cos s \Rightarrow dx = -\sin s \, ds, \]
\[ J = ds/dx = -1/\sin x, \]
\[ g = J^T J = 1/\sin^2 s, \]
\[ g^{11} = g^{-1} = \sin^2 s, \]
\[ |g| = 1/\sin^2 s. \]

By the definition of Laplace-Beltrami operator in (5.2),

\[ \Delta u_{\mathcal{M}} = \frac{1}{|g|} \partial_i (\sqrt{|g|} g^{ij} \partial_j u) \]
\[ = \sin s((1/\sin s) \cdot \sin^2 s \cdot u_x)_x \]
\[ = \sin s(\sin s \cdot u_x)_x, \]

which is exactly the same as the result in (5.8).

The 1D Dirichlet problem

\[ -u_{ss} = \lambda u \text{ in } \mathcal{M} \]
\[ u = 0 \text{ on } \partial\mathcal{M}, \] (5.10)

100
has the solution

\[ u(s) = c_1 \cos(\sqrt{\lambda} s) + c_2 \sin(\sqrt{\lambda} s). \]  
(5.11)

In the Cartesian coordinate system, it is

\[ u(x) = c_1 \cos(\sqrt{\lambda} \cos^{-1}(x)) + c_2 \sin(\sqrt{\lambda} \cos^{-1}(x)), \]  
(5.12)

where \( c_1, c_2 \) are constant coefficients. By applying the boundary conditions,

\[ \begin{align*}
  u(-1) &= c_1 \cos(\sqrt{\lambda} \pi) + c_2 \sin(\sqrt{\lambda} \pi) = 0 \\
  u(1) &= c_1 \cos(\sqrt{\lambda} 0) + c_2 \sin(\sqrt{\lambda} 0) = 0, \quad c_1 = 0 \\
  \Rightarrow & \quad \sin(\sqrt{\lambda} \pi) = 0 \\
  \sqrt{\lambda} \pi &= k\pi, \lambda = k^2, \quad k \in \mathbb{Z}.
\end{align*} \]  
(5.13)

**General formulation**  Consider a general surface \( \mathcal{M} : y = f(x), \quad x \in [a, b] \). The arclength formula is \( ds = \sqrt{1 + (f'(x))^2} \, dx \). Using expression (5.3) for the metric tensor,

\[ \begin{align*}
  J &= \sqrt{1 + (f'(x))^2} \\
  g &= J^T J = 1 + (f'(x))^2 \\
  g^{11} &= 1 / (1 + (f'(x))^2) \\
  |g| &= 1 + (f'(x))^2.
\end{align*} \]  
(5.14)

By the definition of the Laplace-Beltrami operator in (5.2),
\[ \Delta u_M = \frac{1}{\sqrt{|g|}} \partial_1 (\sqrt{|g|} g^{11} \partial_1 u) \]
\[ = \frac{1}{\sqrt{1+(f'(x))^2}} \left( \sqrt{1+(f'(x))^2} \cdot \frac{1}{(1+(f'(x))^2)} \cdot u_x \right)_x \]
\[ = \frac{1}{\sqrt{1+(f'(x))^2}} \left( (1+(f'(x))^2)^{-1/2} \cdot u_x \right)_x \]
\[ = \frac{1}{\sqrt{1+(f'(x))^2}} \left( -\frac{1}{2} (1+(f'(x))^2)^{-3/2} \cdot \frac{f''}{(1+(f'(x))^2)^2} \cdot u_x + (1+(f'(x))^2)^{-1/2} \cdot u_{xx} \right) \]
\[ = -\frac{f''}{(1+(f'(x))^2)^2} u_x + \frac{1}{1+(f'(x))^2} u_{xx}. \] (5.15)

Thus, the general eigenvalue problem is of the form
\[ -\frac{1}{1+(f'(x))^2} u_{xx} + \frac{f''}{(1+(f'(x))^2)^2} u_x = \lambda \rho u. \] (5.16)

In the self-adjoint form,
\[ -\frac{1}{\sqrt{1+(f'(x))^2}} \frac{d}{dx} \left( \frac{u_x}{\sqrt{1+(f'(x))^2}} \right) = \lambda \rho u. \]

**Numerical results** Several numerical results for eigenvalue problems on manifolds will end this subsection. The second-order finite difference method is used to approximate the differential equations. For the following examples, the density function is considered uniform \( \rho = 1 \) on \( M \). The first six eigenvalues and eigenfunctions are shown for each corresponding manifold in Figure 5.1-5.3.

1. Half unit circle determined by (5.6)
\[
\begin{align*}
\lambda_1 &= 1.0043 \\
\lambda_2 &= 4.0173 \\
\lambda_3 &= 9.0389 \\
\lambda_4 &= 16.0691 \\
\lambda_5 &= 25.1079 \\
\lambda_6 &= 36.1554
\end{align*}
\]

Figure 5.1: Solutions on manifold \( \mathcal{M} : \{ (x, y) | y = \sqrt{1 - x^2}, x \in [-1, 1] \} \)

2. Manifold \( \mathcal{M} : \{ (x, y) | y = \sin x + 1, x \in [0, 3\pi] \} \)
Figure 5.2: Solutions on manifold $\mathcal{M} : \{(x, y) | y = \sin x + 1, x \in [0, 3\pi]\}$

3. Manifold $\mathcal{M} : \{(x, y) | y = 3x^4 - 16x^3 + 18x^2, x \in [-1, 4]\}$
Figure 5.3: Solutions on manifold $\mathcal{M} : \{(x, y) | y = 3x^4 - 16x^3 + 18x^2, \ x \in [-1, 4]\}$

5.1.2 Optimization Problem

Next, the optimization problems on manifolds $y = f(x)$ are solved. Consider the equation

$$
- \frac{1}{\sqrt{1 + (f')^2}} \frac{du}{dx} \left( \frac{u}{\sqrt{1 + (f')^2}} \right) = \lambda \rho u \quad \text{in} \quad \Omega, \\
\quad u = 0, \quad \text{on} \quad \partial \Omega,
$$

(5.17)
where $\Omega$ is the projection of the manifold onto the Cartesian coordinate system. Let $D \subset \Omega$ be a subset inside $\Omega$, and do not assume any topology on $D$. Assume the density function $\rho(x)$ takes on two values $0 \leq \rho_1 \leq \rho_2 < \infty$,

$$
\rho(x) = \begin{cases} 
\rho_1 & \text{for } x \in D \\
\rho_2 & \text{for } x \notin D,
\end{cases}
$$

Solve the minimization problem

$$
\min_{\rho(x)} \lambda_k \tag{5.18}
$$

subject to the constraint

$$
\int_{\Omega} \rho dx = K, \tag{5.19}
$$

where $K$ is a prescribed constant. In all the results that follow, $\rho_1 = 1$ and $\rho_2 = 2$, and the manifolds have the same total arclength $\pi$.

1. Manifold $\mathcal{M} : \{(x, y) | y = \sqrt{1-x^2}, x \in [-1, 1]\}$, $K = 3$. Figures 5.4-5.7 show the optimal results and the changes in adjacent eigenvalues for eigenvalues at each iteration step.
$\lambda_1^{(0)} = 0.66151$

$u_1^{(0)}$

$\lambda_1^{(1)} = 0.62826$

$u_1^{(1)}$

$\lambda_1^{(2)} = 0.62666$

$u_1^{(2)}$

$\lambda_1^{(8)} = 0.62648$

$u_1^{(8)}$

$\min_\rho \lambda_1$

$\min_\rho \lambda_1$

$\min_\rho \lambda_1$

$\min_\rho \lambda_1$

Figure 5.4: Profiles of density and eigenfunctions at selected iteration steps when calculating $\min_\rho \lambda_1$ on manifold $\mathcal{M} : \{(x, y) | y = \sqrt{1 - x^2}, x \in [-1, 1]\}$, $K = 3$: Changes in eigenvalues $\lambda_1$ and $\lambda_2$.

Figure 5.4 illustrates the results for $\min_\rho \lambda_1$. The configuration of the density functions and the corresponding eigenfunctions at iterations 0, 1, 2, 8 are shown on the manifold separately. The initial guess for $\min_\rho \lambda_1$ is shown for $\lambda_1^{(0)}$. The
optimal result \((\lambda_1^{(8)})\) indicates that the places with larger density value \(\rho_2\) are in the center, which is consistent with Krein’s theory in 1D Euclidean plane (Theorem 2.3.5 (i)). The third row in Figure 5.4 plots the changes in adjacent eigenvalues \(\lambda_{1-2}\).

Figure 5.5: Profiles of density and eigenfunctions at selected iteration steps when calculating \(\min_{\rho} \lambda_2\) on manifold \(\mathcal{M} : \{(x, y) | y = \sqrt{1 - x^2}, x \in [-1, 1]\}\), \(K = 3\): Changes in eigenvalues \(\lambda_{1-3}\).
Figure 5.5 illustrates the results for $\min_\rho \lambda_2$. The configuration of the density functions and the corresponding eigenfunctions at iterations 0, 1, 2, 11 are shown on the manifold separately. The initial guess for $\min_\rho \lambda_2$ is shown for $\lambda_2^{(0)}$. The optimal result ($\lambda_2^{(11)}$) indicates that the places with larger density value $\rho_2$ have two pieces, each within a bisection of the manifold. This is in close agreement with Krein’s theory in 1D Euclidean plane (Theorem 2.3.5 (ii)). The third row in Figure 5.5 plots the changes in adjacent eigenvalues $\lambda_{1-3}$. 
Figure 5.6: Profiles of density and eigenfunctions at selected iteration steps when calculating $\min_{\rho} \lambda_3$ on manifold $M : \{(x, y) | y = \sqrt{1 - x^2}, x \in [-1, 1]\}$, $K = 3$: Changes in eigenvalues $\lambda_{2-4}$.

Figure 5.6 illustrates the results for $\min_{\rho} \lambda_3$. The configuration of the density functions and the corresponding eigenfunctions at iterations 0, 1, 2, 17 are shown on the manifold separately. The initial guess for $\min_{\rho} \lambda_3$ is shown for $\lambda_3^{(0)}$. The
optimal result \( (\lambda_3^{(17)}) \) indicates that the places with larger density value \( \rho_2 \) have three pieces, each within a trisection of the manifold. This is in close agreement with Krein's theory in 1D Euclidean plane (Theorem 2.3.5 (ii)). The third row in Figure 5.6 plots the changes in adjacent eigenvalues \( \lambda_{2-4} \).

Figure 5.7: Profiles of density and eigenfunctions at selected iteration steps when calculating \( \min_\rho \lambda_4 \) on manifold \( \mathcal{M} : \{ (x, y) | y = \sqrt{1 - x^2}, x \in [-1, 1] \} \), \( K = 3 \): Changes in eigenvalues \( \lambda_{3-5} \).
Figure 5.7 illustrates the results for \( \min_{\rho} \lambda_4 \). The configuration of the density functions and the corresponding eigenfunctions at iterations 0, 1, 2, 4 are shown on the manifold separately. The initial guess for \( \min_{\rho} \lambda_4 \) is shown for \( \lambda_4^{(0)} \). The optimal result \( (\lambda_4^{(4)}) \) indicates that the places with larger density value \( \rho_2 \) have four pieces, each within a quarter section of the manifold. This is in close agreement with Krein’s theory in 1D Euclidean plane (Theorem 2.3.5 (ii)). The third row in Figure 5.7 plots the changes in adjacent eigenvalues \( \lambda_{3-5} \).

2. Manifold \( \mathcal{M} : \{(x, y) | y = \frac{1}{2}(e^x + e^{-x}), \ x \in [0, \ln(\pi + \sqrt{\pi^2 + 1})]\}, \ K = \frac{3}{2} \ln(\pi + \sqrt{\pi^2 + 1}) \). It is easy to verify that the arc length of this manifold is \( \pi \). Figures 5.8-5.11 show the optimal results and the changes in adjacent eigenvalues. It turns out that the optimal results for \( \min_{\rho} \lambda_{1-4} \) are very similar to the results on the manifold of a half circle. However, due to the asymmetry of the manifold, the optimal results are not uniformly distributed.
Figure 5.8: Profiles of density and eigenfunctions at selected iteration steps when calculating \(\min_\rho \lambda_1\) on manifold \(\mathcal{M}\): \(\{(x, y) | y = \frac{1}{2}(e^x + e^{-x}), x \in [0, \ln(\pi + \sqrt{\pi^2 + 1})]\}\), \(K = \frac{3}{2} \ln(\pi + \sqrt{\pi^2 + 1})\): Changes in eigenvalues \(\lambda_1\) and \(\lambda_2\).
Figure 5.9: Profiles of density and eigenfunctions at selected iteration steps when calculating $\min_\rho \lambda_2$ on manifold $\mathcal{M}$: \{(x, y)|y = \frac{1}{2}(e^x + e^{-x}), \ x \in [0, \ln(\pi + \sqrt{\pi^2 + 1})]\}, \ K = \frac{3}{\pi} \ln(\pi + \sqrt{\pi^2 + 1})$: Changes in eigenvalues $\lambda_{1-3}$. 
Figure 5.10: Profiles of density and eigenfunctions at selected iteration steps when calculating $\min_{\rho} \lambda_3$ on manifold $\mathcal{M}$: $\{(x, y)|y = \frac{1}{2}(e^x + e^{-x}), x \in [0, \ln(\pi + \sqrt{\pi^2 + 1})]\}$, $K = \frac{3}{2} \ln(\pi + \sqrt{\pi^2 + 1})$: Changes in eigenvalues $\lambda_{2-4}$. 
Figure 5.11: Profiles of density and eigenfunctions at selected iteration steps when calculating minₚ λ₄ on manifold \( \mathcal{M} \): \( \{(x,y)|y = \frac{1}{2}(e^x + e^{-x}), \ x \in [0, \ln(\pi + \sqrt{\pi^2 + 1})]\} \), \( K = \frac{3}{2} \ln(\pi + \sqrt{\pi^2 + 1}) \): Changes in eigenvalues \( \lambda_{3-5} \).

3. Manifold \( \mathcal{M} \) : \( \{(x,y)|y = x^{3/2}, \ x \in [1, 2.431656]\} \), \( K = 3.647484 \). It is easy to verify that the arc length of this manifold is \( \pi \). Figures 5.12-5.15 show the optimal results and the changes in adjacent eigenvalues. It turns out that the
optimal results for $\min_\rho \lambda_{1-4}$ are also very similar to the results on the manifold of a half circle. This is another example where the optimal results are not uniformly distributed due to the asymmetry of the manifold.

Figure 5.12: Profiles of density and eigenfunctions at selected iteration steps when calculating $\min_\rho \lambda_1$ on manifold $\mathcal{M} : \{(x,y) | y = x^{3/2}, \ x \in [1,2.431656]\}$, $K = 3.647484$: Changes in eigenvalues $\lambda_1$ and $\lambda_2$. 

117
Figure 5.13: Profiles of density and eigenfunctions at selected iteration steps when calculating $\min_p \lambda_2$ on manifold $\mathcal{M} : \{(x, y)|y = x^{3/2}, x \in [1, 2.431656]\}$, $K = 3.647484$: Changes in eigenvalues $\lambda_1-3$. 

\[ \lambda_2^{(0)} = 2.91 \] 
\[ u_2^{(0)} \]
\[ \lambda_2^{(1)} = 2.3432 \] 
\[ u_2^{(1)} \]
\[ \lambda_2^{(2)} = 2.2353 \] 
\[ u_2^{(2)} \]
\[ \lambda_2^{(7)} = 2.189 \] 
\[ u_2^{(7)} \]
Figure 5.14: Profiles of density and eigenfunctions at selected iteration steps when calculating $\min_p \lambda_3$ on manifold $M : \{ (x, y) | y = x^{3/2}, x \in [1, 2.431656] \}$, $K = 3.647484$: Changes in eigenvalues $\lambda_{2-4}$. 
Figure 5.15: Profiles of density and eigenfunctions at selected iteration steps when calculating \( \min_p \lambda_4 \) on manifold \( M : \{(x, y) | y = x^{3/2}, x \in [1, 2.431656] \} \), \( K = 3.647484 \): Changes in eigenvalues \( \lambda_{3-5} \).
5.2 2D problems

General formulation  Consider a general manifold $\mathcal{M}$ in 2D $z = f(x, y)$, $(x, y) \in \Omega$. The arclength formulae are

$$ds = \sqrt{1 + f_x^2} \, dx, \quad dt = \sqrt{1 + f_y^2} \, dy. \quad (5.20)$$

Similar to the derivation in 1D case, we have the Jacobian matrix

$$J = \begin{pmatrix} \sqrt{1 + f_x^2} & 0 \\ 0 & \sqrt{1 + f_y^2} \end{pmatrix} \quad (5.21)$$

the Riemannian metric is

$$g = J^T J = \begin{pmatrix} 1 + f_x^2 & 0 \\ 0 & 1 + f_y^2 \end{pmatrix} \quad (5.22)$$

and the inverse matrix is

$$g^{-1} = \begin{pmatrix} g^{11} & g^{12} \\ g^{21} & g^{22} \end{pmatrix} = \begin{pmatrix} 1/(1 + f_x^2) & 0 \\ 0 & 1/(1 + f_y^2) \end{pmatrix} \quad (5.23)$$

By the definition of the Laplace-Beltrami operator in (5.2),
\[ \Delta u_M = \frac{1}{\sqrt{|g|}} \partial_1(\sqrt{|g|} g^{11} \partial_1 u) + \frac{1}{\sqrt{|g|}} \partial_2(\sqrt{|g|} g^{22} \partial_2 u) \]
\[ = \frac{1}{\sqrt{(1 + f_x^2)(1 + f_y^2)}} \left( \sqrt{(1 + f_x^2)} (1 + f_y^2) \cdot \frac{1}{1 + f_x^2} \cdot u_x \right)_x + \frac{1}{\sqrt{(1 + f_x^2)(1 + f_y^2)}} \left( \sqrt{(1 + f_x^2)} (1 + f_y^2) \cdot \frac{1}{1 + f_y^2} \cdot u_y \right)_y \]
\[ = \frac{1}{\sqrt{(1 + f_x^2)(1 + f_y^2)}} \left( \frac{1 + f_y^2}{1 + f_x^2} \right)^{-1/2} \cdot \frac{f_y f_{yx} (1 + f_y^2) - 2(1 + f_x^2) f_x f_{xx}}{(1 + f_x^2)^2} u_x + \sqrt{1 + f_x^2} u_{xx} \]
\[ + \frac{1}{\sqrt{(1 + f_x^2)(1 + f_y^2)}} \left( \frac{1 + f_x^2}{1 + f_y^2} \right)^{-1/2} \cdot \frac{f_x f_{xy} (1 + f_x^2) - 2(1 + f_y^2) f_y f_{yy}}{(1 + f_y^2)^2} u_y + \sqrt{1 + f_y^2} u_{yy} \]
\[ = \frac{1}{1 + f_x^2} \left[ \left( \frac{f_y f_{yx}}{1 + f_y^2} - \frac{f_x f_{xx}}{1 + f_x^2} \right) u_x + u_{xx} \right] + \frac{1}{1 + f_y^2} \left[ \left( \frac{f_x f_{xy}}{1 + f_x^2} - \frac{f_y f_{yy}}{1 + f_y^2} \right) u_y + u_{yy} \right]. \quad (5.24) \]

Thus, the general eigenvalue problem is of the form
\[ -\frac{1}{1 + f_x^2} \left[ \left( \frac{f_y f_{yx}}{1 + f_y^2} - \frac{f_x f_{xx}}{1 + f_x^2} \right) u_x + u_{xx} \right] - \frac{1}{1 + f_y^2} \left[ \left( \frac{f_x f_{xy}}{1 + f_x^2} - \frac{f_y f_{yy}}{1 + f_y^2} \right) u_y + u_{yy} \right] = \lambda \rho u. \quad (5.25) \]

That is,
\[ -\frac{1}{\sqrt{(1 + f_x^2)(1 + f_y^2)}} \nabla \cdot (c(x, y) \cdot \nabla u) = \lambda \rho u, \quad (5.26) \]
where
\[ c(x, y) = \left( \sqrt{\frac{1 + f_x^2}{1 + f_x^2}}, \sqrt{\frac{1 + f_y^2}{1 + f_y^2}} \right). \quad (5.27) \]

The example chosen to illustrate the numerical solutions is on the top half \( S^2 \) surface
\[ \mathcal{M} : z = f(x, y) = \sqrt{1 - x^2 - y^2}, \quad x^2 + y^2 \leq 1. \quad (5.28) \]
Direct computation gives
\[
c(x, y) = \left( \sqrt{\frac{1-x^2}{1-y^2}}, \sqrt{\frac{1-y^2}{1-x^2}} \right),
\]
\[
\sqrt{(1 + f_x^2) (1 + f_y^2)} = \frac{\sqrt{(1-x^2)(1-y^2)}}{1-x^2-y^2}.
\]
(5.29)

Figure 5.16 shows the first four eigenfunctions of the Dirichlet problem:
\[
-\frac{1}{\sqrt{(1+f_x^2)(1+f_y^2)}} \nabla \cdot (c(x, y) \cdot \nabla u) = \lambda u, \quad \text{in } x^2 + y^2 < 1
\]
\[
u = 0 \quad \text{on } x^2 + y^2 = 1.
\]
(5.30)

Figure 5.16: The eigenfunctions on the manifold \( \mathcal{M} \): \( z = f(x, y) = \sqrt{1-x^2-y^2} \), \( x^2 + y^2 \leq 1 \). 3D and 2D top views are shown for eigenmodes 1-4.

The first row shows the first four eigenfunctions plotted on the top half sphere and the second row shows the top views of them. Since \( \lambda_3 = \lambda_2 \), there is a degeneracy.
and the eigenfunction can be rotated without affecting \( \lambda_2 \). In other words, there is a 1-parameter family of eigenfunctions.

**Numerical results**  This chapter concludes with some optimal results for the top half \( S^2 \) surface (5.28). The governing equation is

\[
-\frac{1}{1+f_x^2} \left[ \left( \frac{f_y f_{xy}}{1+f_y^2} - \frac{f_x f_{yx}}{1+f_x^2} \right) u_x + u_{xx} \right] - \frac{1}{1+f_y^2} \left[ \left( \frac{f_x f_{yy}}{1+f_x^2} - \frac{f_y f_{yx}}{1+f_y^2} \right) u_y + u_{yy} \right] = \lambda \rho u \quad \text{in} \quad \Omega
\]

\[
u = 0 \quad \text{on} \quad \partial \Omega,
\]

where \( \Omega = \{ (x, y) | x^2 + y^2 \leq 1 \} \). The goal is to find

\[
\min_{\rho(x)} \lambda_k
\]

subject to the constraint

\[
\int_{\Omega} \rho \, dx = K,
\]

where \( K \) is a prescribed constant and the density function \( \rho(x) \) takes on two values \( 0 \leq \rho_1 \leq \rho_2 < \infty \),

\[
\rho(x) = \begin{cases} 
\rho_1 & \text{for } x \in D \\
\rho_2 & \text{for } x \notin D.
\end{cases}
\]

For all the numerical results reported here \( \rho_1 = 1, \rho_2 = 2, \) and \( K = \frac{3\pi}{2} \). Figures 5.17-5.20 illustrate the results and the changes in the adjacent eigenvalues during the iteration process. The first row gives the the density functions plotted on the half sphere, the second row gives the 2D top views of them, and the last row plots the changes in the adjacent eigenvalues.
Figure 5.17: Results at selected iteration steps; the region of $\rho_1$ is in cyan, and the region of $\rho_2$ is in magenta. $\min_{\rho} \lambda_1 = 2.6181$.

Figure 5.17 shows the results for $\min_{\rho} \lambda_1$. The optimal result is similar to the result in the 2D Euclidean plane, where larger density values occur in the center. The third row in Figure 5.17 plots the changes in adjacent eigenvalues $\lambda_{1-2}$.
Figure 5.18: Results at selected iteration steps; the region of $\rho_1$ is in cyan, and the region of $\rho_2$ is in magenta. $\min_\rho \lambda_2 = 5.7387$.

Figure 5.18 shows the results for $\min_\rho \lambda_2$. The optimal result indicates that the places with larger density value have two regions, each within a bisection of the manifold. The third row in Figure 5.18 plots the changes in adjacent eigenvalues $\lambda_{1-3}$. Notice
that this optimization process takes much more iterations than other problems. Since there is a rotation symmetry, rotation of a given density distribution does not change the spectral of eigenvalues. During this optimization process, the shape of high-density regions keeps rotating clockwise. However, the second eigenvalue still keeps decreasing. Whenever there are infinite density configurations that have the same eigenvalue, the number of iterations usually increases.
Figure 5.19: Results at selected iteration steps; the region of $\rho_1$ is in cyan, and the region of $\rho_2$ is in magenta. $\min_\rho \lambda_3 = 6.2543$.

Figure 5.19 shows the results for $\min_\rho \lambda_3$. The optimal result indicates that the places with larger density value look like a torus. The third row in Figure 5.19 plots the changes in adjacent eigenvalues $\lambda_{1-4}$. There is a degeneracy at $\lambda_3$, linear combination
\[ \psi = \frac{1}{2}(u_2^2 + u_3^2) \] is used in the sorting process at each step, where \( u_{2-3} \) are the corresponding eigenfunctions.

![Figure 5.20](image-url)

Figure 5.20: Results at selected iteration steps; the region of \( \rho_1 \) is in cyan, and the region of \( \rho_2 \) is in magenta. \( \min \rho \lambda_4 = 9.654 \).
Figure 5.20 shows the results for $\min_\rho \lambda_4$. The optimal result indicates that the places with larger density value have four regions, each within a quarter section of the manifold. The third row in Figure 5.20 plots the changes in adjacent eigenvalues $\lambda_{3-5}$.

### 5.3 Conclusion

In summary, this variational form based numerical approach can be readily extended to more complicated domains and it proves successful in minimizing eigenvalues in the domain of manifolds. The discrete sorting idea allows the piecewise constant distribution of the density function and dramatically decreases the iteration steps. It is useful to conclude the first part of this thesis with some interesting problems for future study. The fourth order elliptic eigenvalue equation describing the vibration of a nonhomogeneous plate is under study in doing the shape optimization of the corresponding plate [14]. The governing eigenvalue equation is

$$\Delta^2 u = \lambda \rho u, \text{ in } \Omega,$$

where $\Delta^2 u = \Delta(\Delta u)$ is the usual biharmonic operator. Depending on whether the boundary is hinged or clamped, the variational form of the equation has different formulations. For example, a clamped plate has the Dirichlet boundary condition:

$$u = \frac{\partial u}{\partial n} = 0, \text{ on } \partial \Omega.$$
The variational form is then

\[ \lambda_k(\rho) = \min_{w \in H^2_0(\Omega)} \frac{\int_{\Omega} (\Delta w)^2 dx}{\int_{\Omega} \rho w^2 dx}, \]  

(5.36)

where \(w\) is orthogonal to \(u_1, \cdots, u_{k-1}\)

where \(u_1, \cdots, u_{k-1}\) are the first \(k-1\) eigenfunctions. The minimum is achieved at the corresponding eigenfunction. Similarly, a hinged plate has the boundary condition:

\[ u = \Delta u = 0, \text{ on } \partial \Omega, \]  

(5.37)

and the associated variational form

\[ \lambda_k(\rho) = \min_{w \in H^2(\Omega) \cap H^1_0(\Omega)} \frac{\int_{\Omega} (\Delta w)^2 dx}{\int_{\Omega} \rho w^2 dx}. \]  

(5.38)

\(w\) is orthogonal to \(u_1, \cdots, u_{k-1}\)

The proposed numerical approach can be directly applied to the optimization problem

\[ \min_{\rho(x)} \lambda_k, \text{ or } \max_{\rho(x)} \lambda_k, \text{ or } \min_{\rho(x)} \frac{\lambda_{k+1}}{\lambda_k}, \]  

(5.39)

where \(\rho(x)\) is a piecewise constant function

\[ \rho(x) = \begin{cases} 
\rho_1 & \text{for } x \in D \\
\rho_2 & \text{for } x \notin D,
\end{cases} \]  

(5.40)

with \(D \subset \Omega\) a bounded subset inside \(\Omega\) and the density function satisfies the fixed mass constraint

\[ \int_{\Omega} \rho(x) dx = K. \]  

(5.41)
Part II

Gyrification Study
CHAPTER 6

INTRODUCTION

This part of the thesis reports the collaborative work on gyrification study of human brain with Tonya White, Marcus Schmidt, Chiu-Yen Kao, and Guillermo Sapiro [60]. Part of this work has been published in [69].

The cortical surface of a human brain evolves from a smooth, or lissencephalic surface, to a highly convoluted surface during the third trimester of fetal life [66]. This process is known as gyrification, and by the time of birth the human brain, although smaller, has an appearance very much like an adult brain. Even though a cortical surface is considered to be a topological sphere, the gyri and sulci that form the fissures and folds can be complicated [66]. It has been suggested that a higher degree of folding of the cortical surface indicates a progressive evolution of cortical complexity in humans [72]. The increased cortical folding associated with human phylogeny has produced a highly efficient mechanism to increase cortical gray matter while optimizing a smaller overall brain size. Cortical complexity, which is considered a measure of gyrification, reveals the general organization in the human cortex and the inherent structural configuration of the brain.

It is of great interest to characterize the surface morphology of the brain, since careful
quantification can provide valuable information associated with alterations or differences related to development and pathology. The cortical complexity has been used to evaluate abnormalities of the brain’s surface morphology in various neurological and psychiatric conditions and in disorders of cognition [68]. Estimates of cortical complexity derived from the number of voxels which occupy the boundary between the gray matter and CSF (cerebral-spinal fluid region) in the prefrontal cortex have shown that abnormalities, such as smaller prefrontal volume, greater sulcal width and gyral pattern abnormalities, are present in first-episode schizophrenia [70]. Since there is a proposed connection between development and gyrification [4], and between gyrification and connectivity [64], these findings may help ascertain the underlying neurobiology of schizophrenia and other psychiatric and neurological disorders.

There is growing interest in how the human brain develops gyri and sulci, how the differences in the degree of convolutions affect brain function, how the cortical folding evolves and whether this evolution is related to human age, gender, ethnicity or health status. These mysteries of human brain development have prompted researchers to develop measurements to quantify the degree of complexity of the cortical surface. The gyrification index (GI) proposed by Zilles et al. [72] was developed to quantify the degree of cortical folding. The GI is defined as the ratio between the total outline (including sulcal folds) and the superficially exposed outline for each coronal section of postmortem brains. Notice that these contours are manually delineated in their proposed method. This GI measure has been applied to study both the phylogeny [72] and ontogeny [4] of cortical gyrification. Brains that have higher degrees of cortical folding (i.e., increased cortical complexity) yield larger values of GI. The anterior to
posterior maps of human GI have shown greater gyrification in the frontal, temporal, and parietal lobes of the brain [72].

However, due to the oblique orientation and manual delineation [72], the intrinsic 3D nature of the brain surface is not taken into account and this gyrification index does not completely avoid a biased estimate. For example, the GI may be altered if the slice orientation is slightly different within the same subject. Since surface morphology can be considered a two-dimensional (2D) surface in three-dimensional (3D) space, it is important to consider a fully 3D gyrification index to eliminate the shortcomings of the coronal 2D approach. Furthermore, manual extraction of the contours is extremely time-consuming and prone to human errors. Thus fully automatic algorithm becomes necessary.

So far, 3D computational algorithms to measure gyrification are based on either curvature or surface area. Curvature-based approaches evaluate the smoothed absolute mean curvature on parameterized cortical mesh models [41, 42, 67]. These curvature based approaches have been shown to find differences which were not previously identified using the traditional GI approach. More recently, a localized 3D gyrification index [55] was developed and applied to a group of children affected by the 22q11.2 Deletion Syndrome. This technique used 3D triangular mesh reconstructions of cortical surfaces and outer hull surfaces, and measured the amount of cortical surface buried in the sulci by constructing and relating this to non-intrinsic spheres with different radii. The authors used the approach developed by Kao et al. [29] to generate the outer hull surface and the localized GI for each point on the cortical surface was obtained through a depth-weighted average of neighboring points. Another approach
was to use the area ratio between the surface area included in a small sphere and the area of a disc of the small radius [62]. Similarly, triangular mesh is used and a non-intrinsic sphere with a suitable radius was constructed at each cortex point. This method turned out to be less sensitive to the choice of different radii. It has been applied to a sample of 314 subjects, 164 females and 150 males. The study showed the disproportionate ratio of cortical surface area to brain size, similar to the earlier observation across species [51]. In addition, the increase of the cortical folding in the prefrontal cortex is observed for larger brains. Since this approach does not require the construction of an outer hull surface, it results in a simple and efficient algorithm compared to the method proposed by [55]. We will further comment on these approaches after we introduce our fully geometric GI measure.

In this part, the goal is to build build upon previous work [29] and propose a 3D geometric approach for the automatic computation of global and regional gyrification indexes of the human brain. By finding a geometrically corresponding region on the outer hull surface for any selected region of interest on the cortical surface, it is possible to define a 3D regional GI as the area ratio between the selected region and the corresponding region of a tightly wrapped sheet around the cortical surface. Furthermore, this 3D GI can be weighted by local quantities, i.e., curvature or geodesic sulcal depth, and is fully intrinsic and different from the method proposed by Schaefer et al. [55] and Toro et al. [62] in that it does not depend on a chosen radius and a corresponding non-intrinsic ball to determine the region used to calculate the localized GI. The incorporation of the robust sulcal depth computation developed in
[29] as part of the GI measurement is important to characterize different levels of convolutions in human brains.

In Section 7, novel algorithms are proposed to calculate 3D gyrification indexes. Quantitative results for our proposed gyrification indexes, and comparison with previous approaches, are presented in Section 8 and this is achieved through the application of the algorithm to a population of typically developing children. Finally, Section 9 concludes with a brief description of the contributions and findings and proposes further lines of study in the area of computational approaches for measuring GI.
CHAPTER 7
MATERIALS AND METHODS

A flow chart explaining the main steps of the proposed 3D geometric GI computation algorithm is shown in Figure 7.1. A triangular mesh of cortical surface shown in Figure 7.1(a) is the input of our algorithm. First, an outer hull surface (see Figure 7.1(b)) covering the sulcal regions in a shrink-wrap fashion is constructed. Second, an efficient fast sweeping algorithm [31, 63, 71] will extract the geodesic depth which will be defined in Section 7.1 (see Figure 7.1(c)). Third, a region on the cortical surface (see Figure 7.1(d)) is selected and its boundary is extracted. Fourth, the corresponding part of the selected region (see Figure 7.1(e)) on the outer hull surface is computed. Fifth and finally, it is possible to define the regional GI as the ratio between the area of the region on the cortical surface and the area of the corresponding region on the outer hull surface. This ratio can be weighted by the local sulcal depth. Each of these steps are explained in detail.
Figure 7.1: Flow chart of the main steps of the proposed GI algorithm. Each figure explains the major steps of the algorithm.
7.1 Surface Extraction and Depth Computation

There are a number of software packages available, e.g., FreeSurfer [15], SurfRelax [35], and BrainVisa [20] to obtain the triangular mesh of cortical surface. In this paper, we used the pial surface generated by FreeSurfer. Meanwhile, total intracranial volume (ICV) was also calculated using the technique developed by Buckner et al. [8]. Let $M$ denote a triangular mesh with faces $f_1, \ldots, f_N$; $M$ is required to be a closed and orientable 2-manifold in Euclidean 3-space. Then a regular grid can be used to derive an implicit representation of the pial surface by computing the signed distance function to the surface on a Cartesian grid [29]. By using a level set technique, an outer hull surface can be computed that encloses the pial surface in a shrink-wrap type fashion. The outer hull is such that one can still distinguish the gyri, but the sulcal regions are now “filled”. A depth measure is then defined for every point on the pial surface as the shortest distance that connects each cortical surface point to a point on the outer hull surface such that the connecting path remains inside the sulcal regions. The computation uses an efficient fast sweeping algorithm.

As shown in Figure 7.1(a), once the explicit form of the pial surface is known, it is possible to compute the signed distance function to the surface on a Cartesian grid. In the implicit form, the pial surface becomes the zero level set $\{\Phi = 0\}$ of the signed

---

1 FreeSurfer, see http://surfer.nmr.mgh.harvard.edu/

2 SurfRelax, see http://www.cns.nyu.edu/~jonas/software.html

3 BrainVisa, see http://brainvisa.info/
distance function $\Phi : \mathcal{R}^3 \rightarrow \mathcal{R}$ [47]. The details for obtaining this signed distance function can be found in [29].

After obtaining both an explicit triangular mesh representation and an implicit level set representation on a Cartesian grid, it is straightforward to compute the outer hull surface using a morphological closing operation applied to the level set function $\Phi$ [47]. That is, first move the pial surface outward by a time parameter $T$, and then we move the surface inward by the same amount of time. The governing equation is

$$
\begin{align*}
\Phi_t + V(t)|\nabla \Phi| &= 0 \\
\Phi(x, y, z, 0) &= \Phi(x, y, z),
\end{align*}
$$

where

$$
V(t) = \begin{cases} 
1, & \text{for } t < T \\
-1, & \text{for } T < t < 2T.
\end{cases}
$$

Thus, the implicit representation of the outer hull surface is given by

$$
\Psi(x) = \min \{\Phi(x, y, z, 2T), \Phi(x, y, z, 0)\}.
$$

This minimization guarantees that the outer hull surface covers, but does not penetrate, the pial surface. In this algorithm, the choice $T = 10$ (mm/unit time) is large enough to fill/close the sulcal regions and also small enough to keep the overall shape of the gyri. Even though the level set method cannot guarantee topology preservation, the numerical implementation shows that the restricted region $\{\Psi \leq 0\}$ is topology preserving. (In case there is a topology change, one can use the topology-preserving level set method [21].) Figure 7.1(b) shows the computed outer hull surface for the given pial surface shown in Figure 7.1(a).
With the generation of the outer hull surface, the fast sweeping method calculates the geodesic depth for points on the pial surface, the geodesic depth corresponds to the shortest path from the given pial surface point to the computed outer hull which do not cross the surface of the brain [29], and thus the distance computation algorithm is restricted to the (CSF) region between the outer hull and the pial surface \( \{ \Psi \leq 0 \text{ and } \Phi \geq 0 \} \). Figure 7.1(c) shows a top view of the bottom part of the pial surface. The color coding corresponds to the computed geodesic depth where shallow regions are colored in blue and deep regions are colored in red.

### 7.2 Computation of the Corresponding Region on the Outer Hull Surface

In this stage, attention is directed to a region of interest (ROI) on the pial surface. The region can be chosen using several different algorithms and can involve any sulcus or gyrus of interest. Alternatively, the region can be restricted by implementing either a depth or curvature threshold. After obtaining the ROI on the pial surface, the corresponding region on the hull surface is computed in two steps.

In the first step, the boundary of the pial surface for the selected region is extracted. This step uses sample points on this boundary and finds the boundary points for the corresponding region on the computed outer hull surface. This is done by following the negative gradient of the previously computed sulcal depth. Paths start at each point situated on the boundary of the selected pial region and satisfy the following
equations:
\[ \frac{dX}{dt} = -\nabla d \]
\[ X(0) = B_p^s \]
\[ X(t) = B_h^s, \]
and the calculation stops at the previously computed outer hull surface. Here \( d \) is the geodesic depth computed in Section 7.1, \( B_p^s \) is a point on the boundary of the selected region on the pial surface, and \( B_h^s \) is then the corresponding boundary point on the outer hull surface. In this way the calculation obtains all the corresponding boundary points on the outer hull surface, in an intrinsic and geometric fashion, and need to close the boundary.

In the second step, connect the computed outer hull boundary points by using the shortest distance along the edges of the triangles. An alternative choice would be to use the geodesic distance on the triangular mesh [50]. Since \( M \) is a closed and orientable 2-manifold in Euclidean 3-space, it is possible to march inside it and find the triangles restricted in the constructed boundary on the outer hull surface.\(^4\) The region defined by these restricted triangles corresponds, on the outer hull surface, to the selected pial region of interest.

Figure 7.1(d) shows a selected region in red on the pial surface, and Figure 7.1(e) shows the computed corresponding region, shown in red on the outer hull surface. Figure 7.2 illustrates the axial, coronal, and sagittal slices of the original MRI brain.

\(^4\)Notice here it is difficult to define the inside/outside for a boundary on a triangular mesh. The good thing is that the triangular mesh is orientable, it is possible to at least obtain one region on the triangular mesh with the extracted boundary by keeping all the triangles the same orientation. Then by comparing this area with the area of the whole outer hull surface, it is possible to determine if the same region or its complement set is the desired set.
volume on which an overlay is shown at the intersection curve of the pial and outer hull surfaces of one hemisphere (in blue) with the selected sulcal region on the pial surface and the computed corresponding region on the outer hull surface (in red). These geometric computations form the basis needed for the gyrification indexes presented next. Before giving the definitions, note that in contrast with [55, 62], where the GI measurements rely on the selection of an extrinsic sphere with predefined radius, this computation of the corresponding outer hull region is completely intrinsic to the geometry of the problem.

7.3 Gyrification Indexes

The most commonly used gyrification index was proposed by Zilles et. al. in 1988 [72], and was defined on each 2D slice \( i \) in the coronal section as the ratio of the length of the total cortical contour \( L^i_T \) to the length of the superficially exposed cortical contour \( L^i_S \), that is,

\[
\text{GI}^i := \frac{L^i_T}{L^i_S},
\]  

(7.5)

the mean GI of each hemisphere was then defined as

\[
\overline{\text{GI}} := \frac{\sum_i L^i_T}{\sum_i L^i_S},
\]  

(7.6)

where the sum runs over all the slices \( i \). This 2D measurement does not allow for the assessment of localized properties, including development of the gyrification. Different theories have postulated that active, localized growth of the cortical convolutions may lead to different brain structures, e.g., regions which are developing into gyri grow
Figure 7.2: Axial (1st column), coronal (2nd column), and sagittal (3rd column) slices of the MRI brain volume combined with the pial and outer hull surfaces of one hemisphere (blue lines). The red part on the curve is the intersection of the selected region (frontal lobe here) on the pial surface and the corresponding region on the outer hull surface. Top three slices correspond to Figure 1(d) (pial surface) and bottom three slices correspond to Figure 1(e) (outer hull).
at a faster rate than areas destined to become sulci. Furthermore, recent research
demonstrates that the development of different regions of the brain may result in
remarkably different brain functioning, e.g., the temporal lobe is more vulnerable due
to preterm births, with a resulting increased temporal lobe GI [33]. Thus, reliable
and accurate regional gyrification indexes are of great interest in the understanding
of the complexity of brain folding.

A. Area-Based Gyrification Measurement

In the following, several gyrification index measurements will be introduced. Using
Freesurfer, each hemisphere is classified into 35 different sulcal and gyral regions, and
a complete labeling of these 35 regions can be obtained by the automated parcellation
system. Group these ROIs into six regions of the human cortex (see Table 7.1 and
note that only 33 regions are involved in the classification): frontal lobe, parietal lobe,
temporal lobe, medial temporal lobe, occipital lobe, and the cingulate gyrus. Figure
7.3 shows the classification of the 6 regions on the left pial surface. It is possible to
successfully identify the corresponding 6 regions on the hull surface. In comparison,
Freesurfer generates the inflated left pial surface as shown in Figure 7.3. The region-
based gyrification index at each lobe is then defined as the ratio between the area of
the lobe on the pial surface and the area of the corresponding region on the outer
hull surface,

$$GI^l_{region} := \frac{A^s_p}{A^p_h}.$$  (7.7)
where \( A_p \) is the area of any selected lobe on the pial surface and \( A_h \) is the corresponding area on the hull surface, computed as detailed in the previous section. This regional gyrification index \( G_{region}^1 \) has several key features:

<table>
<thead>
<tr>
<th>Lobe Type</th>
<th>Regions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frontal Lobe (F)</td>
<td>caudalmiddlefrontal, lateralorbitofrontal,</td>
</tr>
<tr>
<td></td>
<td>medialorbitofrontal, paracentral, parsopercularis,</td>
</tr>
<tr>
<td></td>
<td>parsorbitalis, parstriangularis, precentral,</td>
</tr>
<tr>
<td></td>
<td>rostralmiddlefrontal, superiorfrontal, frontalpole.</td>
</tr>
<tr>
<td>Parietal Lobe (P)</td>
<td>inferiorparietal, postcentral, precuneus,</td>
</tr>
<tr>
<td></td>
<td>superiorparietal, supramarginal.</td>
</tr>
<tr>
<td>Temporal Lobe (T)</td>
<td>bankssts, inferiortemporal, middletemporal,</td>
</tr>
<tr>
<td></td>
<td>superiortemporal, temporalpole, transversetemporal.</td>
</tr>
<tr>
<td>Medial Temporal Lobe (MT)</td>
<td>entorhinal, fusiform, parahippocampal.</td>
</tr>
<tr>
<td>Occipital Lobe (O)</td>
<td>cuneus, lateralocipital, lingual, pericalcarine.</td>
</tr>
<tr>
<td>Cingulate Cortex (C)</td>
<td>caudalanteriorcingulate, isthmuscingulate,</td>
</tr>
<tr>
<td></td>
<td>posteriorcingulate, rostralanteriorcingulate.</td>
</tr>
</tbody>
</table>

Table 7.1: Lobe mapping from the labelling of sulcal and gyral regions.
Figure 7.3: 6 regions of interest on left pial surface (1st column), inflated left pial surface (2nd column), and the left hull surface (3rd column). Frontal lobe is shown in blue, parietal lobe in yellow, temporal lobe in green, medio temporal lobe in cyan, occipital lobe in red, and cingulate cortex in magenta. The region which is not classified is shown in brown.
1. The corresponding region on the outer hull surface is naturally computed from the ROI on the pial surface, leading to a parameter free intrinsic GI. If the whole pial surface is selected, the corresponding region is then the whole outer hull surface. The gyrification index measurement becomes

$$\text{GI}_{\text{global}} = \frac{A_p}{A_h}, \quad (7.8)$$

where $A_p$ is the area of the whole pial surface, and $A_h$ is the area of the whole outer hull surface. If one only considers a slice of the pial surface, the surface area in 3D becomes the slice perimeter in 2D. However, this reduction may still be different from the exact definition of Zilles [72], since the corresponding point on the outer hull surface may not be on the same plane any longer. From this point of view, powerful 3D gyrification index computation is of great importance.

2. Since all the triangles in the selected region on the pial surface are collected, all the sulcal information restricted to the selected area is considered.

3. The selection of the region on the pial surface can be further parceled to determine GIs for different subregions. For instance, having calculated the depth information for each point on the pial surface, it is possible to define a threshold $d_0$ and choose a region of interest as all the points with depth $d \geq d_0$. Other possible choices are to select one of the 35 sulcal or gyral regions as ROI.
B. Depth-Based Gyrification Measurement

Before an extension of the gyrification index $G_{\text{region}}^d$ to a weighted gyrification index by adding the depth information of the pial surface, it is useful to introduce a normalization of the computed depth value.

Since the absolute depth significantly depends on brain size, it is reasonable to consider the relative depth. In this way, two brains with a similar morphology, but different volumes, would have comparable gyrification indices. The implementation uses

$$d_N := \frac{d}{3V/A},$$

where the denominator $3V/A$ on the right hand side is a normalization factor based on volume $V$ and area $A$ [52]. This normalization can be examined by considering a sphere of radius $R$, then the normalized value for a certain depth $d$ of folding becomes

$$d_N = \frac{d}{\frac{\frac{4}{3}\pi R^3}{(4\pi R^2)}} = \frac{d}{\frac{R}{2}},$$

and if the radius is $2R$ and the depth is $2d$, the normalized depth becomes

$$d_N = \frac{2d}{\frac{\frac{4}{3}\pi (2R)^3}{(4\pi (2R)^2)}} = \frac{d}{R}.$$

While these two spheres have similar folding but different depths, the normalized depths are the same.

Remark 1: The human brain is actually more like an ellipsoid elongated on the anterior-posterior direction. So represent the brain surface by an ellipsoid in an $xyz$-Cartesian coordinate system and obtain the equatorial radii $a$ and $b$ (along the $x$
and \( y \) axes) and the polar radius \( c \) (along the \( z \)-axis). The approximate surface area formula (Knud Thomsen’s formula) is

\[
A \approx 4\pi \left( \frac{a^p b^p + a^p c^p + b^p c^p}{3} \right)^{1/p}
\]  

(7.12)

with \( p \approx 1.6075 \). The volume formula of an ellipsoid is

\[
V = \frac{4}{3} \pi abc.
\]

(7.13)

Thus the previously defined normalization factor becomes

\[
\frac{3V}{A} = \frac{\frac{4\pi abc}{4\pi \left( \frac{a^p b^p + a^p c^p + b^p c^p}{3} \right)^{1/p}}}{\frac{abc}{\left( \frac{a^p b^p + a^p c^p + b^p c^p}{3} \right)^{1/p}}}
\]

and this is consistent with a sphere by choosing

\[
R = \frac{abc}{\left( \frac{a^p b^p + a^p c^p + b^p c^p}{3} \right)^{1/p}}.
\]

(7.15)

Now it is possible to define the depth-based gyrification index. For any region \( R_p \) selected on the pial surface, the corresponding region on the outer hull surface is denoted by \( R_h \). A gyrification index that considers the normalized depth information \( d_N \) can be defined as

\[
\text{GI}^2_{\text{region}} := \frac{\sum_{i=1}^{N_p} d_N A_p^i}{\sum_{j=1}^{N_h} A_h^j}
\]

\[
= \frac{\sum_{i=1}^{N_p} d_N A_p^i}{\sum_{i=1}^{N_p} A_p^i} \cdot \frac{A_p^i}{A_h^j} = \frac{\sum_{i=1}^{N_p} d_N A_p^i}{\sum_{i=1}^{N_p} A_p^i} \cdot \text{GI}^1_{\text{region}},
\]

(7.16)
Figure 7.4: Area definition at a vertex in a triangular mesh. For the vertex at the center (cyan), the area is defined as the total area of the region shown in magenta, which is made up of all the triangles constructed by connecting the vertex (cyan), the centroid (black) of its neighboring triangle and the middle point (yellow) of its neighboring ring in the same triangle.

where $N_p$ and $N_h$ are the total number of triangular vertices inside the regions $R_p$ and $R_h$ respectively, $d_N^i$ is the normalized depth of the vertex $i$ (depth to the outer hull surface as detailed before [29], $A_p^i$ is the area of the vertex $i$ in $R_p$, and $A_h^j$ is the area of the vertex $j$ in $R_h$. Notice that $A_p^i$ and $A_h^j$ are defined as before in Section 7.3 A. The area at a vertex $i$ (see Figure 7.4, cyan colored vertex) is defined in the following way. For each neighboring triangle of vertex $i$, find the centroid (see Figure 7.4, black colored) and for each neighboring ring of vertex $i$, find the middle point (see Figure 7.4, yellow colored). Then the area at vertex $i$ is the area sum of all such triangles formed by the vertex $i$, the centroid of the neighboring triangle and the middle point of the neighboring ring in the same triangle. Figure 7.4 illustrates this.
By adding weights to the depth of the pial surface, \( \text{Gi}^2_{\text{region}} \) is in fact a measurement of the average geodesic depth in the selected region of interest on the pial surface scaled by the ratio of the area of the selected region on the pial surface to the area of the corresponding region on the outer hull surface, i.e., \( \text{Gi}^1_{\text{region}} \). Similar to the previously defined gyrification index, the global counterpart of becomes

\[
\text{Gi}^2_{\text{region}} = \frac{\sum_{i \in \text{pial}} d_N^i \cdot A_p^i}{\sum_{j \in \text{outer hull}} A_h^j}. 
\]

(7.17)

This is an approximation of the scaled average geodesic depth of the restricted (CSF) region between the outer hull and the pial surface \( \{ \Psi \leq 0 \text{ and } \Phi \geq 0 \} \).

The rationale behind a measure that is weighted by the geodesic depth is to account for specific differences in brain size, which are different than controlling for ICV alone. In theory, a GI does not need correction, as it is a unitless measure, being either a ratio of distances or a ratio of areas, however, larger brains may contain equal amounts of gray matter, but have less cortical depth. Control for cortical depth effectively uses a complementary technique to evaluate the data.

Remark 2: The localized GI proposed by Schae et al. [55] is obtained through a depth-weighted average of localized GI of the neighboring points. Therefore, this pointwise gyrification index is in fact still region-based since the ROI is defined by the radius of the non-intrinsic sphere.
7.4 Subjects

To study the development of gyrification, the method is implemented on brains from a sample of 26 typically developing children and adolescents. Subjects were stratified into three age groups, which included children (8 to 12 years old), young adolescents (13 to 15 years old), and older adolescents (16 to 19 years of age). The demographic information for the children is provided in Table 7.2. Socioeconomic status was determined using the Four Factor Index of Social Status [24].

<table>
<thead>
<tr>
<th></th>
<th>8 to 12</th>
<th>13 to 15</th>
<th>16 to 19</th>
<th>p</th>
</tr>
</thead>
<tbody>
<tr>
<td>Age</td>
<td>10.5 (1.6)</td>
<td>14.0 (0.87)</td>
<td>16.9 (1.2)</td>
<td></td>
</tr>
<tr>
<td>Sex (Male / Female)</td>
<td>4 / 2</td>
<td>6 / 3</td>
<td>4 / 7</td>
<td>n.s.</td>
</tr>
<tr>
<td>Socioeconomic Status</td>
<td>50.7 (9.7)</td>
<td>49.7 (15.5)</td>
<td>51.1 (9.7)</td>
<td>n.s.</td>
</tr>
</tbody>
</table>

Table 7.2: Demographic information for the 26 typically developing children between the ages of 8 and 19 years of age.

7.5 Statistical Analyses

Evaluation of the differences in demographics was assessed using either one-way ANOVA or t-tests for continuous data and chi-square tests for categorical data. Paired
t-tests were used to assess lateralization of gyrification and cortical depth measures. If gyrification of each hemisphere proceeds independently, then measures for the right and left hemispheres should not be pooled, even if they do not show lateralizing effects. If they are dependent, then they may or may not show lateralization. Since it is not possible to test all of these variables, and since there were differences in lateralization, data from the two hemispheres is not pooled. An ANCOVA of the total sample (14 males and 12 females), with age and ICV as a covariate, was used to evaluate sex effects of sulcal depth. Measures of gyrification were evaluated between the three age groups using a one-way ANOVA.
CHAPTER 8

EXPERIMENTAL RESULTS

8.1 Demographics

There were no differences between the sex, socioeconomic status, or handedness between any of the three age groups (Table 7.2). In addition, when stratified into two groups by sex, there were no differences in the demographic data. An ANCOVA with age as a covariate demonstrated sex differences in the total intracranial volume ($F_{1,23} = 4.8, p = 0.04$), however, there were no differences in ICV between the three age groups.

8.2 Data Analyses on the Pial Surface

Before analyzing the data in detail, it is worth considering an overview of the area ratio and average normalized depth for each lobe on the pial surface. The six regions are shown in Figure 7.3, marked with different colors. Figure 8.1(a) plots the area ratio $A^s_p/A_p$ and Figure 8.1(b) plots the normalized average depth $\left(\sum_{i=1}^{N_p} d_{N_p}^i A_p^i / A_p\right) / A_p$ for each lobe in both hemispheres for all subjects. Here, the notations are the same as mentioned in Chapter 7. Table 8.1 lists the mean value of the area ratio (columns
2 & 3) and the normalized average depth (columns 6 & 7) for all the subjects. They both show no significant intrinsic differences in the left and right hemispheres.

<table>
<thead>
<tr>
<th>Lobe</th>
<th>Area Ratio</th>
<th></th>
<th></th>
<th>Average Depth</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LH (pial surf)</td>
<td>RH (pial surf)</td>
<td>LH (hull surf)</td>
<td>RH (hull surf)</td>
</tr>
<tr>
<td>F</td>
<td>0.3509</td>
<td>0.3533</td>
<td>0.3750</td>
<td>0.3777</td>
</tr>
<tr>
<td>P</td>
<td>0.2265</td>
<td>0.2302</td>
<td>0.1937</td>
<td>0.1909</td>
</tr>
<tr>
<td>T</td>
<td>0.1540</td>
<td>0.1482</td>
<td>0.1527</td>
<td>0.1489</td>
</tr>
<tr>
<td>MT</td>
<td>0.0484</td>
<td>0.0441</td>
<td>0.0634</td>
<td>0.0598</td>
</tr>
<tr>
<td>O</td>
<td>0.1125</td>
<td>0.1164</td>
<td>0.1180</td>
<td>0.1261</td>
</tr>
<tr>
<td>C</td>
<td>0.0364</td>
<td>0.0380</td>
<td>0.0509</td>
<td>0.0507</td>
</tr>
</tbody>
</table>

Table 8.1: Average area ratio on the pial surface, average area ratio of each corresponding region on the hull surface for each lobe, and the mean value of the normalized average depth.
Figure 8.1: Data analyses on the pial surface. Left hemisphere measurements are marked by ‘+’, and right hemisphere measurements are marked by ‘*’.
8.3 Data Analyses on the Outer Hull Surface

The mean value of the area ratio $A_h^r/A_h$ for the corresponding region of each lobe on the outer hull surface are shown in Figure 8.2 and Table 8.1 (columns 4 & 5). As expected, there are no significant differences between the hemispheres and the corresponding order is the same as for the pial surface. They are ordered from the largest to smallest region: frontal lobe, parietal lobe, temporal lobe, occipital lobe, medial temporal lobe, and cingulate cortex.

8.4 Lateralization of Sulcal Depth and Gyrification Measures

A paired $t$-test found that there was significant laterality for the maximum depth for many of the major sulci. These laterality differences are shown in Table 8.2. As expected, the regions which demonstrate lateralizing effects are related to language regions in the temporal lobes, as well as sulci within the frontal and parietal lobes. Sulci that do not show lateralizing effects include areas related to sensory and motor functions (central sulcus and calcarine fissure). Due to these differences, lateralized measures were not pooled to assess for developmental differences in sulcal depth.
Figure 8.2: Area ratio of the corresponding region (area on the hull surface for corresponding ROI/hull surface area) for each region on both hemispheres for all subjects. Left hemisphere measurements are marked by ‘+’, and right hemisphere measurements are marked by ‘*’.
<table>
<thead>
<tr>
<th>Sulci</th>
<th>Maximum Depth (left)</th>
<th>Maximum Depth (right)</th>
<th>t / p</th>
</tr>
</thead>
<tbody>
<tr>
<td>Central Sulcus</td>
<td>29.8 (2.4)</td>
<td>30.1 (2.4)</td>
<td>n.s.</td>
</tr>
<tr>
<td>Lateral Sulcus</td>
<td>34.1 (2.1)</td>
<td>33.5 (1.9)</td>
<td>2.5 / 0.02</td>
</tr>
<tr>
<td>Superior Frontal</td>
<td>20.1 (1.6)</td>
<td>19.2 (2.2)</td>
<td>2.1 / 0.05</td>
</tr>
<tr>
<td>Superior Temporal</td>
<td>22.6 (2.2)</td>
<td>24.8 (2.2)</td>
<td>-7.5 / &lt;0.0001</td>
</tr>
<tr>
<td>Middle Temporal</td>
<td>14.2 (1.9)</td>
<td>15.5 (2.1)</td>
<td>-2.6 / 0.02</td>
</tr>
<tr>
<td>Intraparietal</td>
<td>26.0 (1.7)</td>
<td>26.0 (2.1)</td>
<td>n.s.</td>
</tr>
<tr>
<td>Transverse Occipital</td>
<td>17.2 (1.9)</td>
<td>16.4 (2.3)</td>
<td>n.s.</td>
</tr>
<tr>
<td>Calcarine Fissure</td>
<td>20.2 (3.2)</td>
<td>20.8 (3.5)</td>
<td>n.s.</td>
</tr>
<tr>
<td>Superior Parietal</td>
<td>13.3 (1.7)</td>
<td>14.3 (1.3)</td>
<td>-2.9 / 0.008</td>
</tr>
<tr>
<td>Parieto-occipital Fissure</td>
<td>18.8 (2.6)</td>
<td>20.5 (2.6)</td>
<td>-2.9 / 0.007</td>
</tr>
<tr>
<td>Supramarginal</td>
<td>21.9 (2.2)</td>
<td>21.1 (3.6)</td>
<td>n.s.</td>
</tr>
<tr>
<td>Orbitofrontal</td>
<td>9.6 (1.3)</td>
<td>10.8 (1.0)</td>
<td>-4.7 / &lt;0.0001</td>
</tr>
<tr>
<td>Ant. Ascending Ramus</td>
<td>29.7 (2.8)</td>
<td>27.3 (2.2)</td>
<td>4.8 / &lt;0.0001</td>
</tr>
<tr>
<td>Ant. Horizontal Ramus</td>
<td>13.3 (1.7)</td>
<td>16.2 (3.3)</td>
<td>18.5 / &lt;0.0001</td>
</tr>
</tbody>
</table>

Table 8.2: Maximum depth (in mm) for the major sulci by hemisphere and paired t-test showing lateralization.

Specific brain regions show lateralization in function, such as language centers in the temporal lobe and visuospatial performance in the parietal lobe. In addition,
hemispheric differences in gyrification has also been found in psychiatric disorders [46, 54]. Tests were conducted on whether differences in lateralization were also present in measures of gyrification. Paired t-tests found no differences in either GI\textsuperscript{1}\textsubscript{region} or GI\textsuperscript{2}\textsubscript{region} between the left and right frontal and temporal lobes. However, there were significant laterality effects of both GI\textsuperscript{1}\textsubscript{region} and GI\textsuperscript{2}\textsubscript{region} in the parietal lobe (GI\textsuperscript{1}\textsubscript{region}: t = 4.8, df = 28, p < 0.0001; GI\textsuperscript{2}\textsubscript{region}: t = 2.9, df = 28, p = 0.007), the occipital lobe (GI\textsuperscript{1}\textsubscript{region}: t = 4.6, df = 28, p < 0.0001; GI\textsuperscript{2}\textsubscript{region}: t = 4.6, df = 28, p = 0.01), and the cingulate cortex (GI\textsuperscript{1}\textsubscript{region}: t = 3.3, df = 28, p = 0.004; GI\textsuperscript{2}\textsubscript{region}: t = 2.2, df = 28, p = 0.03). The parietal lobe had greater cortical complexity in the right hemisphere, whereas the occipital lobe and cingular cortex had greater cortical complexity in the left hemisphere. In addition, laterality effects were found in the medial temporal lobes for GI\textsuperscript{2}\textsubscript{region} (t = -2.4, df = 28, p = 0.02), with the left lobe having greater gyrification than the right. Due to these differences, gyrification measures were not pooled for the right and left hemispheres.

8.5 Developmental Differences in Sulcal Depth

There were relatively few differences in sulcal depth between the different age groups for the 15 major sulci that were evaluated. There were age-related differences in the maximum depth of the right middle temporal sulcus ($F_{2,21} = 4.1, p = 0.03$), right lateral sulcus ($F_{2,21} = 3.5, p = 0.05$), and a trend for the right central sulcus ($F_{2,21} = 3.2, p = 0.06$).
8.6 Developmental Differences in Gyrification

There were no differences in the measures of GI_{region}^1 or GI_{region}^2 between males and females in any of the regions of interest, thus these measures were pooled for the analyses. Age-related differences in gyrification for in the left and right hemispheres can be seen in Figure 8.3(a) and Figure 8.3(b), respectively. The GI_{region}^1 decreases with age in the left ($F_{2,24} = 4.6$, $p = 0.02$) and right ($F_{2,24} = 4.9$, $p = 0.02$) frontal lobe; left ($F_{2,24} = 4.2$, $p = 0.03$) and right ($F_{2,24} = 6.8$, $p = 0.004$) medial temporal lobe. In addition, there are trend decreases in the GI_{region}^1 by age in the left ($F_{2,24} = 2.6$, $p = 0.09$) and right parietal ($F_{2,24} = 2.6$, $p = 0.09$).

Fewer age-related differences were found using the gyrification measure which accounts for regional differences in sulcal depth (GI_{region}^2). Age-related differences were found in the left ($F_{2,24} = 4.1$, $p = 0.03$) and right ($F_{2,24} = 6.5$, $p = 0.006$) medial temporal lobe. In addition, trend differences were found in the left ($F_{2,24} = 3.1$, $p = 0.07$) and right ($F_{2,24} = 2.8$, $p = 0.08$) cingulate, left parietal lobe ($F_{2,24} = 2.7$, $p = 0.09$), and the left ($F_{2,24} = 2.5$, $p = 0.10$) and right ($F_{2,24} = 3.3$, $p = 0.06$) frontal lobes.

8.7 Comparison with Existing Techniques

In comparison with the recently proposed 3D GI measurements [55, 62], our proposed GI computation method is parameter free and defines the regional 3D gyrification index directly on the pial surface. In [55], they redistribute the localized gyrification index to any vertex point on the pial surface by first defining the localized gyrification index on the outer hull surface, and the weighting during redistribution is
Figure 8.3: Developmental differences between gyrification indexes within different regions for the both hemispheres.
related to the distance between the vertex point on the pial surface and the involved vertex points on the outer hull surface. There are several possible disadvantages of this method: first of all, the outer hull surface is a surface generated from the pial surface, and strictly speaking, there is no gyrification index on the outer hull surface. Secondly, the extrinsic distance they use in the weighting is along the normal axis of the vertex to the outer hull surface, while our intrinsic distance is the computed geodesic depth [29], which is a more natural technique in defining the gyrification index. In addition, after Schaefer et al. [55] extract the perimeter on the region of interest on the outer hull surface, they project this perimeter to the pial surface by taking the nearest point on the pial surface, whereas our correspondence relies once again on the natural geodesic depth direction. Finally, the results from a spherical mask [55, 62] will depend on the radius used. Smaller spheres will have greater variability secondary to anatomical differences, whereas larger spheres will not provide a localized enough measure of gyrification and will cross boundaries into alternate regions. Nevertheless, the approaches by Schaefer et al. (2008) and Toro et al. (2008) are significant improvements over the previous 2D GI.

A comparison of the technique in this thesis with the localized gyrification index proposed by Schaefer et al. [55] experimentally can be made by calculating localized GI values at different radii and averaged these values into the six defined brain regions. It turns out that localized GI is quite sensitive to the selection of the radius of the sphere. (Radii of 20, 25, 30, and 35 mm as proposed are tested.) With radii of less than 20 mm, not all data could be processed using Freesurfer with a resultant loss in
the degrees of freedom. Table 8.3 lists the one-way ANOVA results for radius of 20, 25, 30, and 35 mm respectively.

A one-way ANOVA test (Table 8.3) illustrates this strong radii dependency. From Table 8.4 one can observe significant differences between radii in the frontal, parietal, and temporal lobes in both hemispheres for the three age groups. Analysis using gender as a covariate shows more variability while the proposed measures GI$_1^{region}$ and GI$_2^{region}$ are more stable. A more complete idea of the effects of the localized GI can be established by a four-radius by three-age-group by two-region ANOVA test, which showed that there were significant effects due to radius ($F_{3,1271} = 44.61$, $p < 0.0001$) and age group ($F_{2,1271} = 19.03$, $p < 0.0001$), but no significant effects due to region ($F_{1,1271} = 1.11$, $p = 0.29$).

### 8.8 Discussion

A novel gyrification index computational technique proves successful in demonstrating developmental differences in gyrification in a cohort of typically developing children and adolescents. The proposed computational method employed intrinsic 3D measurement to find gyrification indexes for a region of interest. It is thus able to identify regional alterations in brain surface complexity.

The results support continued molding of the surface morphology of the brain through childhood and adolescence. This same time period has been shown to be associated with a decrease in surface GM and an associated increase in the surface cerebral spinal fluid [18, 58]. It is not surprising that decreases in the underlying volume of GM would
<table>
<thead>
<tr>
<th>Brain Region</th>
<th>LGI r=20</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Left</td>
<td>Right</td>
<td>Left</td>
<td>Right</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$F_{2.23}/p$</td>
<td>$F_{2.22}/p$</td>
<td>$F_{2.24}/p$</td>
<td>$F_{2.24}/p$</td>
</tr>
<tr>
<td>Frontal</td>
<td>5.7/0.01</td>
<td>3.1/0.07</td>
<td>2.7/0.09</td>
<td>2.5/0.10</td>
<td>3.4/0.05</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Parietal</td>
<td>9.1/0.001</td>
<td>5.2/0.01</td>
<td>7.7/0.003</td>
<td>3.0/0.07</td>
<td>6.1/0.007</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temporal</td>
<td>5.1/0.01</td>
<td>4.5/0.02</td>
<td>3.2/0.06</td>
<td>2.5/0.10</td>
<td>2.6/0.10</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Medial Temporal</td>
<td>0.4/0.7</td>
<td>4.5/0.02</td>
<td>0.3/0.7</td>
<td>1.6/0.2</td>
<td>0.5/0.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Occipital</td>
<td>2.2/0.1</td>
<td>1.5/0.3</td>
<td>2.5/0.1</td>
<td>1.5/0.2</td>
<td>2.9/0.07</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cingulate</td>
<td>5.8/0.009</td>
<td>3.7/0.04</td>
<td>4.7/0.02</td>
<td>4.6/0.02</td>
<td>4.3/0.03</td>
</tr>
</tbody>
</table>

Table 8.3: One-way ANOVA test showing developmental differences between localized GI (LGI) for different radius (mm) within different regions.
<table>
<thead>
<tr>
<th>Brain Region</th>
<th>Agegroup (8-12)</th>
<th></th>
<th>Agegroup (13-15)</th>
<th></th>
<th>Agegroup (16-19)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Left</td>
<td>Right</td>
<td>Left</td>
<td>Right</td>
<td>Left</td>
<td>Right</td>
</tr>
<tr>
<td></td>
<td>$F_{3.20}/p$</td>
<td>$F_{3.20}/p$</td>
<td>$F_{3.35}/p$</td>
<td>$F_{3.35}/p$</td>
<td>$F_{3.40}/p$</td>
<td>$F_{3.30}/p$</td>
</tr>
<tr>
<td>Frontal</td>
<td>9.1/0.0005</td>
<td>11.5/0.0001</td>
<td>7.7/0.0004</td>
<td>8.1/0.0003</td>
<td>6.5/0.001</td>
<td>10.9/0</td>
</tr>
<tr>
<td>Parietal</td>
<td>11.3/0.0001</td>
<td>6.4/0.003</td>
<td>5.8/0.002</td>
<td>10.0/0</td>
<td>6.5/0.001</td>
<td>11.8/0</td>
</tr>
<tr>
<td>Temporal</td>
<td>6.6/0.003</td>
<td>9.3/0.0005</td>
<td>6.9/0.001</td>
<td>9.96/0</td>
<td>7.4/0.0005</td>
<td>19.8/0</td>
</tr>
<tr>
<td>Medial Temporal</td>
<td>0.06/0.98</td>
<td>0.3/0.8</td>
<td>0.23/0.9</td>
<td>1.6/0.2</td>
<td>0.3/0.8</td>
<td>0.2/0.9</td>
</tr>
<tr>
<td>Occipital</td>
<td>1.8/0.2</td>
<td>1.0/0.4</td>
<td>0.13/0.9</td>
<td>2.1/0.1</td>
<td>0.49/0.7</td>
<td>0.5/0.7</td>
</tr>
<tr>
<td>Cingulate</td>
<td>1.5/0.3</td>
<td>0.76/0.5</td>
<td>0.98/0.4</td>
<td>1.3/0.3</td>
<td>2.3/0.1</td>
<td>2.1/0.1</td>
</tr>
</tbody>
</table>

Table 8.4: One-way ANOVA test showing differences of localized GI between radius (mm) for each age group in each region.
result in an associated decrease in cortical complexity, as has been demonstrated in typically developing adults [42]. The developmental differences in GI are localized to the later maturing structures, including the frontal and medial temporal lobes [27, 25]. Regions that develop earlier, such as the occipital, parietal, and lateral temporal lobes, do not demonstrate the same level of developmental differences as the frontal and medial temporal regions [26].

The brain has reached its peak volume by eight years of age and thus it is not surprising that there are not striking developmental differences in the depths of the major sulci. Indeed, the primary sulci are the first to develop and are associated with a greater heritability [40]. The secondary and tertiary sulci develop later, and are more linked to environmental factors. However, most of the primary and secondary sulci form during the third trimester of fetal life [66] and it is likely that restructuring and depth of the major sulci, including laterality differences, are fairly stable by eight years of age. Future studies mapping the development of the sulci, gyri and GI between birth and eight years of age will be beneficial to assess alterations of these measures as language and other cognitive processes mature.

There are limitations to the current study. In particular, the sample size to evaluate for developmental differences is relatively small. However, the fact that significant findings were present and were consistent across measures may reflect a relatively robust measure to assess developmental differences.
CHAPTER 9
CONCLUDING REMARKS AND DISCUSSION

The 3D geometric approach presented in this thesis for defining the global and regional gyrification indexes naturally extends the standard way of defining the coronal 2D GI and fully utilizes the intrinsic 3D nature of human cortical surface. Classifying the cortical surface into 6 different regions and defining a simple regional gyrification index on each region as the area ratio of corresponding surfaces helps us to more carefully characterize the cortical complexity in each region and therefore provides a better way to understand the effect of each region in brain functioning. Furthermore, applying the method in a clinical study, the proposed measurement of depth-weighted regional gyrification turns out to be more robust in finding the developmental differences in children and adolescents, e.g., the results show significantly increased gyrification in the right parietal lobe and right cingulate cortex, as well as age-rated differences in the left frontal, right parietal and the right cingulate cortex. These findings provide some references for future study of the relationship between gyrification and neurological and psychiatric conditions, in addition to the development of other more advanced techniques to quantify the gyrification of the human brain.

Since there is not one universally accepted definition for computational GI, and this
is a relatively new and ongoing research area, it is useful to conclude this discussion
with some possible alternatives that deserve further study.

From a statistical point of view, the 3D regional gyrification index $GI^2_{\text{region}}$ is essent-
ially an estimation of the first moment of the area. This motivates a consideration
of higher order moments. For instance, a second central moment estimator

$$GI^3_{\text{region}} = \frac{\sum_{i=1}^{N_p} (d_N^i - d_0) \cdot A_p^i}{\sum_{j=1}^{N_h} A_h^j},$$

(9.1)

where

$$d_0 = \frac{\sum_{i=1}^{N_p} d_N^i \cdot A_p^i}{\sum_{i=1}^{N_p} A_p^i},$$

(9.2)

is the average depth in the selected region and, evaluates the variance of the area
distribution and the third central moment estimator will then help in evaluating the
skewness of the area distribution.

The gyrification index measurement does not necessarily need to be a scalar value, so
it is possible to also consider a vectorized gyrification index measurement. For any
selected region $R_p$ on the pial surface and the corresponding region on the outer hull
surface, define (for example)

$$GI^4_{\text{region}} = \overline{GI}_{\text{region}} := \begin{bmatrix} GI^1_{\text{region}} & GI^2_{\text{region}} \end{bmatrix}$$

$$= \begin{bmatrix} A_p \cdot \frac{\sum_{i=1}^{N_p} d_N^i \cdot A_p^i}{\sum_{j=1}^{N_h} A_h^j} \\
\end{bmatrix}.$$  

(9.3)
This expression allows an evaluation of the local sulci information considering both the area ratio and the average depth of the selected region, narrowing the similarity between different regions and providing more information for analyzing the brain complexity.

In summary, a novel approach has been presented to measure 3D gyrification of the human brain and have applied this measure to evaluate age-related differences in typically developing adolescents. Developmental differences in gyrification were readily detected between childhood and young adulthood (Figure 8.3) as well as different trajectories between the different brain lobes. Future studies are needed that evaluating longitudinal assessments of gyrification may provide greater resolution of the age related changes. In addition, test-retest studies of individuals who are learning a specific task (i.e., playing a musical instrument) would be beneficial to determine if specific regions change with practice. It is possible that measures of GI are more sensitive to subtle changes in GM compared to volume measures.

The use of lobar regions of interest that were applied can reduce the structural variability compared to techniques which utilize voxel-based moving-average measures. Nevertheless, a ‘gold standard’ measure for GI does not currently exist and a study performing a ‘head-to-head’ assessment of the different approaches for measuring GI would be beneficial. The findings here suggest that brain gyrification continues to change from childhood through young adulthood.
Appendix A

SOLUTIONS TO THE ELLIPTIC EIGENVALUE PROBLEMS

Six elliptic eigenvalue problems are solved exactly to provide tests of the algorithms described in Chapter 3. The details follow.

1. Dirichlet Problem

Consider the problem

\[-\Delta u(x, y) = \lambda u(x, y) \quad \Omega = [0, 1] \times [0, 1], \]
\[u(x, y) = 0 \quad \partial \Omega. \]  \hspace{1cm} (A.1)

Assume that \(u(x, y)\) can be expressed as a product of a function of \(x\) and a function \(y\). Thus, seek a solution of the form

\[u(x, y) = T(x)S(y).\]

After differentiating,

\[-T''(x)S(y) - T(x)S''(y) = \lambda T(x)S(y), \]  \hspace{1cm} (A.2)

and dividing by the product \(T(x)S(y)\), (A.2) becomes

\[-\frac{T''}{T} - \frac{S''}{S} = \lambda. \]  \hspace{1cm} (A.3)
Since the first term on the left hand side of the above equation is a function of \( x \) and the second term on the left hand side is a function of \( y \) alone, this can only happen when each terms equals a constant. Thus,

\[
\begin{align*}
\frac{T''}{T} &= \tau_1 \\
T(0) &= T(1) = 0 \\
\frac{S''}{S} &= \tau_2 \\
S(0) &= S(1) = 0 \\
\lambda &= \tau_1 + \tau_2.
\end{align*}
\]  \hspace{1cm} \text{(A.4)}

Now the problem becomes two one-dimensional problems and the solutions are

\[
\begin{align*}
T &= C_1 \sin\left(\sqrt{\tau_1}x\right), & C_1 \text{ constant} \\
\tau_1 &= (k\pi)^2, & k \in \mathbb{Z}. \\
S &= C_2 \sin\left(\sqrt{\tau_2}y\right), & C_2 \text{ constant} \\
\tau_2 &= (l\pi)^2, & l \in \mathbb{Z}. \\
u(x, y) &= C \sin(k\pi x) \sin(l\pi y), & C \text{ constant} \\
\lambda &= (k\pi)^2 + (l\pi)^2, & k, l \in \mathbb{Z}.
\end{align*}
\]  \hspace{1cm} \text{(A.5)}

The first nine eigenvalues are

\[
(2, 5, 5, 8, 10, 10, 13, 13, 17) \pi^2.
\]  \hspace{1cm} \text{(A.6)}

2. Neumann Problem

Consider the problem

\[
\begin{align*}
-\Delta u(x, y) &= \lambda u(x, y) & \Omega = [0, 1] \times [0, 1], \\
\frac{\partial u}{\partial n} &= 0 & \partial \Omega.
\end{align*}
\]  \hspace{1cm} \text{(A.7)}
By separation of variables,

\[-\frac{T''}{T} = \tau_1\]
\[T'(0) = T'(1) = 0\]
\[-\frac{S''}{S} = \tau_2\]
\[S'(0) = S'(1) = 0\]
\[\lambda = \tau_1 + \tau_2.\]  \hfill (A.8)

Solving the above two one-dimensional equations,

\[T = C_1 \cos(\sqrt{\tau_1}x), \quad C_1 \text{ constant}\]
\[\tau_1 = (k\pi)^2, \quad k \in Z.\]

\[S = C_2 \cos(\sqrt{\tau_2}y), \quad C_2 \text{ constant}\]
\[\tau_2 = (l\pi)^2, \quad l \in Z.\]

\[u(x, y) = C \cos(k\pi x) \cos(l\pi y), \quad C \text{ constant}\]
\[\lambda = (k\pi)^2 + (l\pi)^2, \quad k, l \in Z.\]  \hfill (A.9)

Thus, the first nine positive eigenvalues are

\[(1, 1, 2, 4, 4, 5, 8, 9) \pi^2 \]  \hfill (A.10)

3. Robin Problem

Consider the problem

\[-\Delta u(x, y) = \lambda u(x, y) \quad \Omega = [0, 1] \times [0, 1],
\]
\[\frac{\partial u}{\partial n} + u = 0 \quad \partial \Omega. \]  \hfill (A.11)
By separation of variables,

\[-\frac{T''}{T'} = \tau_1\]
\[T(0) - T'(0) = 0\]
\[T(1) + T'(1) = 0\]
\[-\frac{S''}{S} = \tau_2\]
\[S(0) - S'(0) = 0\]
\[S(1) + S'(1) = 0\]
(\[\lambda = \tau_1 + \tau_2.\]

Solving the above two one-dimensional equations,

\[T = C_1 \cos(\sqrt{\tau_1}x) + C_2 \sin(\sqrt{\tau_1}x),\]
\[S = C_3 \cos(\sqrt{\tau_2}y) + C_4 \sin(\sqrt{\tau_2}y),\]
\[u(x,y) = (C_1 \cos(\sqrt{\tau_1}x) + C_2 \sin(\sqrt{\tau_1}x))(C_3 \cos(\sqrt{\tau_2}y) + C_4 \sin(\sqrt{\tau_2}y)),\]
\[\lambda = \tau_1 + \tau_2,\]
(A.13)

where \(C_1, C_2, C_3, C_4\) are constants, \(\tau_1, \tau_2\) are solutions of the equation

\[f(\tau) = 2\sqrt{\tau} + (1 - \tau) \tan \sqrt{\tau} = 0.\]
(A.14)

The first several numerical solutions for this nonlinear equation are

\[\tau = 1.7071, 13.492, 43.357.\]
(A.15)

Thus, the first nine eigenvalues are

\[\lambda_1 = 3.4141, \quad \lambda_4 = 26.985, \quad \lambda_7 = 56.850,\]
\[\lambda_2 = 15.199, \quad \lambda_5 = 45.064, \quad \lambda_8 = 56.850,\]
\[\lambda_3 = 15.199, \quad \lambda_6 = 45.064, \quad \lambda_9 = 86.714.\]
(A.16)
4. Dirichlet Problem with Variable Coefficient

Consider the problem

\[-\Delta u(x, y) = \lambda \rho(x) u(x, y) \quad \Omega = [0, 1] \times [0, 1], \]
\[u = 0 \quad \partial \Omega,\]

where

\[\rho(x) = \begin{cases} 1 & x \in [0, \frac{1}{2}), \\ 2 & x \in (\frac{1}{2}, 1]. \end{cases} \]

By separation of variables,

\[\frac{T''}{T} + \lambda \rho(x) = -\frac{S''}{S}, \]

Notice that the left hand side of the above equation depends on \( x \) whereas the right hand side depends only on \( y \). This can only happen when both equal to a constant. Thus,

\[\frac{T''}{T} + \lambda \rho(x) = C\]
\[T(0) = T(1) = 0\]
\[-\frac{S''}{S} = C\]
\[S(0) = S(1) = 0,\]

where \( C \) is a constant. The solution for \( S(y) \) is

\[S = a_1 \sin(\sqrt{C}y), \quad a_1 \text{ constant}\]
\[C = (k\pi)^2, \quad k \in \mathbb{Z}.\]
The problem for $T(x)$ is

$$T'' + (\lambda - C)T = 0 \quad \text{in } (0, \frac{1}{2})$$
$$T'' + (2\lambda - C)T = 0 \quad \text{in } (\frac{1}{2}, 1)$$

(A.22)

$$T(0) = T(1) = 0.$$

Assuming $\lambda > 0$ and $T > 0$, there are three possibilities:

(I) $2\lambda - C > \lambda - C > 0$

$$T(x) = \begin{cases} 
  a_2 \sin \sqrt{\lambda - C} x & \text{in } (0, \frac{1}{2}) \\
  a_3 \sin \sqrt{2\lambda - C} (x - 1) & \text{in } (\frac{1}{2}, 1),
\end{cases}$$

(A.23)

where $a_2, a_3$ are constant coefficients. The continuity conditions for $T$ and $T'$ at $\frac{1}{2}$ give the relations

$$a_2 \sin \sqrt{\frac{\lambda - C}{2}} = -a_3 \sin \sqrt{\frac{2\lambda - C}{2}},$$

$$a_2 \sqrt{\lambda - C} \cos \sqrt{\frac{\lambda - C}{2}} = a_3 \sqrt{2\lambda - C} \cos \sqrt{\frac{2\lambda - C}{2}},$$

(A.24)

which is equivalent to the equation

$$\frac{\tan \sqrt{\frac{\lambda - C}{2}}}{\tan \sqrt{\frac{2\lambda - C}{2}}} = -\frac{\sqrt{\lambda - C}}{\sqrt{2\lambda - C}}.$$  

(A.25)

(II) $2\lambda - C > 0 > \lambda - C$

$$T(x) = \begin{cases} 
  a_4 \sinh \sqrt{C - \lambda} x & \text{in } (0, \frac{1}{2}) \\
  a_5 \sin \sqrt{2\lambda - C} (x - 1) & \text{in } (\frac{1}{2}, 1),
\end{cases}$$

(A.26)

where $a_4, a_5$ are constant coefficients. The equation for this case is then

$$\frac{\tanh \sqrt{\frac{C - \lambda}{2}}}{\tan \sqrt{\frac{2\lambda - C}{2}}} = -\frac{\sqrt{C - \lambda}}{\sqrt{2\lambda - C}}.$$  

(A.27)
(III) \(0 > 2\lambda - C > \lambda - C \)

\[ T(x) = \begin{cases} 
    a_6 \sinh \sqrt{C - \lambda}x & \text{in } (0, \frac{1}{2}) \\
    a_7 \sinh \sqrt{C - 2\lambda(x - 1)} & \text{in } (\frac{1}{2}, 1),
\end{cases} \tag{A.28}
\]

where \(a_6, a_7\) are constant coefficients. The equation for this case is then

\[ \frac{\tanh \frac{\sqrt{C - \lambda}}{2}}{\tanh \frac{\sqrt{C - 2\lambda}}{2}} = -\frac{\sqrt{C - \lambda}}{\sqrt{C - 2\lambda}}. \tag{A.29} \]

After solving the nonlinear equations for \(\lambda\), the first nine eigenvalues are

\[
\begin{align*}
\lambda_1 & = 12.516, & \lambda_4 & = 56.297, & \lambda_7 & = 86.964, \\
\lambda_2 & = 29.649, & \lambda_5 & = 58.265, & \lambda_8 & = 91.737, \\
\lambda_3 & = 35.976, & \lambda_6 & = 65.541, & \lambda_9 & = 92.225.
\end{align*}
\tag{A.30}
\]

5. Neumann Problem with Variable Coefficient

Consider the problem

\[
-\Delta u(x, y) = \lambda \rho(x) u(x, y) \quad \Omega = [0, 1] \times [0, 1],
\]

\[
\frac{\partial u}{\partial n} = 0 \quad \partial \Omega,
\tag{A.31}
\]

where

\[
\rho(x) = \begin{cases} 
    1 & x \in [0, \frac{1}{2}), \\
    2 & x \in (\frac{1}{2}, 1].
\end{cases} \tag{A.32}
\]

By separation of variables,

\[
\frac{T''}{T} + \lambda \rho(x) = -\frac{S''}{S}, \tag{A.33}
\]

179
Notice that the left hand side of the above equation depends on $x$ whereas the right hand side depends only on $y$. This can only happen when both equal to a constant. Thus,

\[
\frac{T''}{T} + \lambda \rho(x) = C
\]

\[T'(0) = T'(1) = 0\]  \hspace{1cm} \text{(A.34)}

\[-\frac{S''}{S} = C\]

\[S'(0) = S'(1) = 0,\]

where $C$ is a constant. The solution for $S(y)$ is

\[S = a_1 \cos(\sqrt{C} y), \quad a_1 \text{ constant} \] \hspace{1cm} \text{(A.35)}

\[C = (k\pi)^2, \quad k \in \mathbb{Z}.\]

The problem for $T(x)$ is

\[T'' + (\lambda - C)T = 0 \quad \text{in } (0, \frac{1}{2})\]

\[T'' + (2\lambda - C)T = 0 \quad \text{in } (\frac{1}{2}, 1)\] \hspace{1cm} \text{(A.36)}

\[T'(0) = T'(1) = 0.\]

Assuming $\lambda > 0$ and $T > 0$, there are three possibilities:

(I) $2\lambda - C > \lambda - C > 0$

\[T(x) = \begin{cases} 
    a_2 \cos \sqrt{\lambda - C} x & \text{in } (0, \frac{1}{2}) \\
    a_3 \cos \sqrt{2\lambda - C} (x - 1) & \text{in } (\frac{1}{2}, 1),
\end{cases} \] \hspace{1cm} \text{(A.37)}

where $a_2, a_3$ are constant coefficients. The continuity conditions for $T$ and $T'$ at $\frac{1}{2}$ give the relations

\[a_2 \cos \frac{\sqrt{\lambda - C}}{2} = a_3 \cos \frac{\sqrt{2\lambda - C}}{2},\]

\[-a_2 \sqrt{\lambda - C} \sin \frac{\sqrt{\lambda - C}}{2} = a_3 \sqrt{2\lambda - C} \sin \frac{\sqrt{2\lambda - C}}{2}, \] \hspace{1cm} \text{(A.38)}

180
which is equivalent to the equation
\[ \sqrt{\lambda - C} \tan \frac{\sqrt{\lambda - C}}{2} + \sqrt{2\lambda - C} \tan \frac{\sqrt{2\lambda - C}}{2} = 0. \] (A.39)

(II) \( 2\lambda - C > 0 > \lambda - C \)
\[
T(x) = \begin{cases} 
  a_4 \cosh \sqrt{C - \lambda} x & \text{in } (0, \frac{1}{2}) \\
  a_5 \cos \sqrt{2\lambda - C} (x - 1) & \text{in } (\frac{1}{2}, 1),
\end{cases} \tag{A.40}
\]
where \( a_4, a_5 \) are constant coefficients. The equation for this case is then
\[ \sqrt{C - \lambda} \tanh \frac{\sqrt{C - \lambda}}{2} - \sqrt{2\lambda - C} \tan \frac{\sqrt{2\lambda - C}}{2} = 0. \] (A.41)

(III) \( 0 > 2\lambda - C > \lambda - C \)
\[
T(x) = \begin{cases} 
  a_6 \cosh \sqrt{C - \lambda} x & \text{in } (0, \frac{1}{2}) \\
  a_7 \cosh \sqrt{C - 2\lambda} (x - 1) & \text{in } (\frac{1}{2}, 1),
\end{cases} \tag{A.42}
\]
where \( a_6, a_7 \) are constant coefficients. The equation for this case is then
\[ \sqrt{C - \lambda} \tanh \frac{\sqrt{C - \lambda}}{2} + \sqrt{C - 2\lambda} \tan \frac{\sqrt{C - 2\lambda}}{2} = 0. \] (A.43)

After solving the nonlinear equations for \( \lambda \), the first nine positive eigenvalues are
\[
\begin{align*}
\lambda_1 &= 6.0967, & \lambda_4 &= 22.073, & \lambda_7 &= 39.478, \\
\lambda_2 &= 7.1691, & \lambda_5 &= 25.819, & \lambda_8 &= 47.343, \\
\lambda_3 &= 15.273, & \lambda_6 &= 32.312, & \lambda_9 &= 53.531. \tag{A.44}
\end{align*}
\]

181
6. Robin Problem with Variable Coefficient

Consider the problem

\[-\Delta u(x, y) = \lambda \rho(x) u(x, y) \quad \Omega = [0, 1] \times [0, 1],\]  
\[\frac{\partial u}{\partial n} + u = 0 \quad \partial \Omega,\]  

where

\[\rho(x) = \begin{cases} 
1 & x \in [0, \frac{1}{2}), \\
2 & x \in (\frac{1}{2}, 1]. 
\end{cases}\]  

By separation of variables,

\[\frac{T''}{T'} + \lambda \rho(x) = -\frac{S''}{S},\]  

Notice that the left hand side of the above equation depends on \(x\) whereas the right hand side depends only on \(y\). This can only happen when both equal to a constant. Thus,

\[\frac{T''}{T'} + \lambda \rho(x) = C\]  
\[T(0) - T'(0) = 0\]  
\[T(1) + T'(1) = 0\]  
\[-\frac{S''}{S} = C\]  
\[S(0) - S'(0) = 0\]  
\[S(1) + S'(1) = 0,\]  

where \(C\) is a constant. The solution for \(S(y)\) is

\[S = a_1 \cos \sqrt{C} y + a_2 \sin \sqrt{C} y, \quad a_1, a_2 \text{ constants,}\]  

where \(C\) is the solution of the equation

\[f(\tau) = 2\sqrt{\tau} + (1 - \tau) \tan \sqrt{\tau} = 0.\]
The first several numerical solutions for this nonlinear equation are

\[ \tau = 1.7071, 13.492, 43.357, 92.769. \quad (A.51) \]

The problem for \( T(x) \) is

\[
\begin{align*}
T'' + (\lambda - C)T &= 0 \quad \text{in} \ (0, \frac{1}{2}) \\
T'' + (2\lambda - C)T &= 0 \quad \text{in} \ (\frac{1}{2}, 1) \\
T(0) - T'(0) &= 0 \\
T(1) + T'(1) &= 0.
\end{align*}
\]

(A.52)

Assuming \( \lambda > 0 \) and \( T > 0 \), there are three possibilities:

(I) \( 2\lambda - C > \lambda - C > 0 \)

\[
T(x) = \begin{cases} 
  a_3 \cos \sqrt{\lambda - C}x + a_4 \sin \sqrt{\lambda - C}x & \text{in} \ (0, \frac{1}{2}) \\
  a_5 \cos \sqrt{2\lambda - C}(x - 1) + a_6 \sin \sqrt{2\lambda - C}(x - 1) & \text{in} \ (\frac{1}{2}, 1),
\end{cases}
\]

(A.53)

where \( a_3, a_4, a_5, a_6 \) are constant coefficients. The boundary conditions and the continuity conditions for \( T \) and \( T' \) at \( \frac{1}{2} \) give the relations

\[
\begin{align*}
  a_3 - a_4 \sqrt{\lambda - C} &= 0, \\
  a_5 + a_6 \sqrt{2\lambda - C} &= 0, \\
- a_3 \sqrt{\lambda - C} \sin \frac{\sqrt{\lambda - C}}{2} &= a_4 \sqrt{\lambda - C} \cos \frac{\sqrt{\lambda - C}}{2} \\
= a_5 \sqrt{2\lambda - C} \sin \frac{\sqrt{2\lambda - C}}{2} &= a_6 \sqrt{2\lambda - C} \cos \frac{\sqrt{2\lambda - C}}{2},
\end{align*}
\]

(A.54)
which after some manipulation, is equivalent to the equation

\[
\frac{\sqrt{\lambda-C} \cos \frac{\sqrt{\lambda-C}}{2} + \sin \frac{\sqrt{\lambda-C}}{2}}{(\lambda-C) \sin \frac{\sqrt{\lambda-C}}{2} - \sqrt{\lambda-C} \cos \frac{\sqrt{\lambda-C}}{2}} + \frac{\sqrt{2\lambda-C} \cos \frac{\sqrt{2\lambda-C}}{2} + \sin \frac{\sqrt{2\lambda-C}}{2}}{(2\lambda-C) \sin \frac{\sqrt{2\lambda-C}}{2} - \sqrt{2\lambda-C} \cos \frac{\sqrt{2\lambda-C}}{2}} = 0.
\]

(A.56)

(II) \(2\lambda - C > 0 > \lambda - C\)

\[
T(x) = \begin{cases} 
  a_7 \cosh \sqrt{C-\lambda} x + a_8 \sinh \sqrt{C-\lambda} x & \text{in } (0, \frac{1}{2}) \\
  a_9 \cos \sqrt{2\lambda-C} (x-1) + a_{10} \sin \sqrt{2\lambda-C} (x-1) & \text{in } (\frac{1}{2}, 1), 
\end{cases}
\]

(A.57)

where \(a_7, a_8, a_9, a_{10}\) are constant coefficients. The equation for this case is then

\[
\frac{\sqrt{C-\lambda} \cosh \frac{\sqrt{C-\lambda}}{2} + \sinh \frac{\sqrt{C-\lambda}}{2}}{(C-\lambda) \sinh \frac{\sqrt{C-\lambda}}{2} + \sqrt{C-\lambda} \cosh \frac{\sqrt{C-\lambda}}{2}} + \frac{\sqrt{2\lambda-C} \cosh \frac{\sqrt{2\lambda-C}}{2} + \sinh \frac{\sqrt{2\lambda-C}}{2}}{(2\lambda-C) \sinh \frac{\sqrt{2\lambda-C}}{2} + \sqrt{2\lambda-C} \cosh \frac{\sqrt{2\lambda-C}}{2}} = 0.
\]

(A.58)

(III) \(0 > 2\lambda - C > \lambda - C\)

\[
T(x) = \begin{cases} 
  a_{11} \cosh \sqrt{C-\lambda} x + a_{12} \sinh \sqrt{C-\lambda} x & \text{in } (0, \frac{1}{2}) \\
  a_{13} \cosh \sqrt{2\lambda-C} (x-1) + a_{14} \sinh \sqrt{2\lambda-C} (x-1) & \text{in } (\frac{1}{2}, 1), 
\end{cases}
\]

(A.59)

where \(a_{11}, a_{12}, a_{13}, a_{14}\) are constant coefficients. The equation for this case is then

\[
\frac{\sqrt{C-\lambda} \cosh \frac{\sqrt{C-\lambda}}{2} + \sinh \frac{\sqrt{C-\lambda}}{2}}{(C-\lambda) \sinh \frac{\sqrt{C-\lambda}}{2} + \sqrt{C-\lambda} \cosh \frac{\sqrt{C-\lambda}}{2}} + \frac{\sqrt{2\lambda-C} \cosh \frac{\sqrt{2\lambda-C}}{2} + \sinh \frac{\sqrt{2\lambda-C}}{2}}{(2\lambda-C) \sinh \frac{\sqrt{2\lambda-C}}{2} + \sqrt{2\lambda-C} \cosh \frac{\sqrt{2\lambda-C}}{2}} = 0.
\]

(A.60)
After solving the nonlinear characteristic equations for $\lambda$, the first nine eigenvalues are

\[
\begin{align*}
\lambda_1 &= 2.2206, & \lambda_4 &= 20.837, & \lambda_7 &= 37.560, \\
\lambda_2 &= 9.2533, & \lambda_5 &= 25.327, & \lambda_8 &= 44.102, \\
\lambda_3 &= 11.197, & \lambda_6 &= 29.614, & \lambda_9 &= 50.715.
\end{align*}
\]
BIBLIOGRAPHY


