AMATH 563: COMPUTATIONAL REPORT 4

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1. Introduction

In this report, we will use a specific construction of the graph Laplacian operator to approximate the Laplacian differential operator on the unit box. Specifically, we want to verify the eigenvectors of the graph Laplacian converge to the eigenfunction on a Neumann eigenvalue problem. To measure the convergence, we will compare the subspace the eigenvectors and the eigenfunction span. In addition to the unit box, the eigenvector of the Laplacian will be considered over an irregular L shape domain.

2. Methods

Consider the unit box domain $\Omega = [0,1]^2$ and a graph with the dataset $G = (X, W)$ where $X = \{x_1, ..., x_m\}$ is the set of m uniformly distributed random points and W is a specific weight matrix that represents the distance between each point. Each point $x_i \in X$ corresponds to a spatial pair (x, y) that denotes its position in Ω. Define the weight matrix $W \in \mathbb{R}^{mxm}$ as the following

$$w_{ij} = k_\epsilon(||x_i - x_j||_2), \qquad \text{where } k_\epsilon(||x_i - x_j||_2) = \begin{cases} (\pi\epsilon^2)^{-1}, & ||x_i - x_j||_2 \le \epsilon \\ 0 & ||x_i - x_j||_2 > \epsilon \end{cases}$$

where $||x_i - x_j||_2$ is the pairwise Euclidean distance, the parameter $\epsilon > 0$ controls the local connectivity of the graph G; if the pair of node are within a ϵ neighborhood, then they have a non-zero weight. In this report, we choose $\epsilon(m) = C\frac{\log)m)^{\frac{3}{4}}}{m^{\frac{1}{2}}}$ where $C > 0$ is a constant and m is the number of points distributed in Ω.

Given W, define the diagonal degree matrix D as

$$D = \text{diag}(d) \qquad \text{where } d = (d_1, .., d_m)^T \text{ and } d_i = \sum_j^m W_{ij}$$

In other words, the entries of a degree matrix are the sum of the weights associated with each $x_i \in X$. Then, we have the unnormalized graph Laplacian matrix $L = D - W$ of G. Fixing the number of points in Ω to be $m = 2048$, we convert the graph Laplacian matrix L into a sparse matrix for computational efficiency and use the eigsh function from scipy.sparse.linalg to find the first 4 eigenvectors $\mathbf{q_1}, ..., \mathbf{q_4} \in \mathbb{R}^m$ with the smallest magnitude and their corresponding eigenvalue. We will examine the four eigenvectors as functions over Ω.

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To compare the graph Laplacian matrix with the differential Laplacian operator $\mathcal{L}$, define the continuous operator as acting on some function $f : \Omega \to \mathbb{R}$ and $f \in C^2(\Omega)$ as

$$\mathcal{L}f = -(\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2})$$

and consider the Neumann eigenvalue problem $\begin{cases} \mathcal{L}\psi = \lambda(n,k)\psi & \text{in } \Omega \\ \nabla\psi \cdot \mathbf{n} = 0 & \text{on } \partial\Omega \end{cases}$ where the eigenvalue λ depends on the mode n, k and $\mathbf{n}$ is the outward normal vector on the boundary $\partial\Omega$. By separation of variables, we are given the solution $\psi(\mathbf{x}) = \cos(n\pi x_1)\cos(k\pi x_2)$ where $\mathbf{x} = (x_1, x_2)^T$.

Define the $j-$th normalized and discretized eigenfunction as $\boldsymbol{\psi}_j \in \mathbb{R}^m$ as

$$\boldsymbol{\psi}_j = \frac{\tilde{\boldsymbol{\psi}}}{||\tilde{\boldsymbol{\psi}}||_2}$$

where $\tilde{\boldsymbol{\psi}} \in \mathbb{R}^m$ contains the values of the first four eigenfunction $\psi(x)$ at $m = 2048$ points of $x_i \in X$ and the modes $(n,k) = (0,0), (0,1), (1,0), (1,1)$.

To verify the convergence of the graph Laplacian matrix eigenvector and the Neumann eigenfunction over Ω, we choose to show that the $\text{span}\{\mathbf{q}_1, ..., \mathbf{q}_4\} \approx \text{span}\{\boldsymbol{\psi}_1, ..., \boldsymbol{\psi}_4\}$. Now choosing $m = \{2^7, 2^5, ..., 2^{10}\}$, we will generate m number of points in the unite box and compute $\epsilon(m)$, $\mathbf{q}_1, ..., \mathbf{q}_4$, and $\psi_1, ..., \psi_4$ for each m. Then, define the following matrices

$$Q := [\mathbf{q}_1|, ..., |\mathbf{q}_4] \in \mathbb{R}^{mx4} \qquad \Psi := [\psi_1|, ..., |\boldsymbol{\psi}_4] \in \mathbb{R}^{mx4}$$

where the projectors onto the subspace spanned by the vectors $\mathbf{q}_i$ and $\boldsymbol{\psi}_i$ can be defined as $P_Q = QQ^T$ and $P_\Psi = \Psi\Psi^T$. We now can compute the absolute error for each m by examining the commutativity of the projectors given

$$\text{error}(m) := ||P_Q P_\Psi - P_\psi P_Q||_F$$

where $||\cdot||_F$ denotes the Frobenius norm.

To test the performance of the graph Laplacian to approximate the eigenfunction of the differential Laplacian operator, consider the irregular L-shape domain $\Omega = ([0,1]^2) \cup ([1,2] \times [0,1]) \cup ([0,1] \times [1,2])$. Let $m = 2^{13} = 8192$ and generate the set of m uniformly random points X, we will compute $\epsilon(m)$ to find the eigenvectors $\mathbf{q}_7, ..., \mathbf{q}_{10}$ of L.

3. Results

1 shows the first four smallest eigenvector of the graph Laplacian L as functions over Ω where the color represents the values of the eigen vector entry and the coordinate (x, y) reveals the spatial coordinate in the unit box. 2 shows the first four eigenfunction with the mode $(n,k) = (0,0), (0,1), (1,0), (1,1)$. Both plot was generated on a uniformly distributed random set of 2048 points. It is evident that the graph Laplacian adequately approximated the values of the eigenfunction up to visual accuracy as the color gradient, of which corresponds to the function values, is similar for the second, third, and fourth eigenvector. While both graphs have slight color variation, the color for the smallest eigenvector $\mathbf{q}_1$ plot is not consistent with the smallest Neumann eigenfunction with the node $(0,0)$. This inconsistency could be due to the smallest eigenvalue being close to machine precision, a reflection of round-off errors.

Beyond the visual accuracy, 3 shows the average error between the subspaces $\text{span}\{\mathbf{q}_1, ..., \mathbf{q}_4\}$ and $\text{span}\{\boldsymbol{\psi}_1, ..., \boldsymbol{\psi}_4\}$ over 30 trials for $m = \{2^7, 2^5, ..., 2^{10}\}$. As seen on the graph, the average error decreases as the number of points in X increases. In other words, the subspace of the eigenvector $\text{span}\{\mathbf{q}_1, ..., \mathbf{q}_4\}$ seems to converge to the subspace of the eigenfunction $\text{span}\{\boldsymbol{\psi}_1, ..., \boldsymbol{\psi}_4\}$ as m increases.

4 shows the first four smallest eigenvectors of the graph Laplacian L on an L-shape domain. For an irregular domain like $\Omega = ([0,1]^2) \cup ([1,2] \times [0,1]) \cup ([0,1] \times [1,2])$, solving for the eigenfunction analytically can be difficult. Here there are no eigenfunction to compare the precisions of the eigenvectors $\mathbf{q}_7, ..., \mathbf{q}_{10}$, nevertheless the graph Laplacian can still be tested on irregular domains.

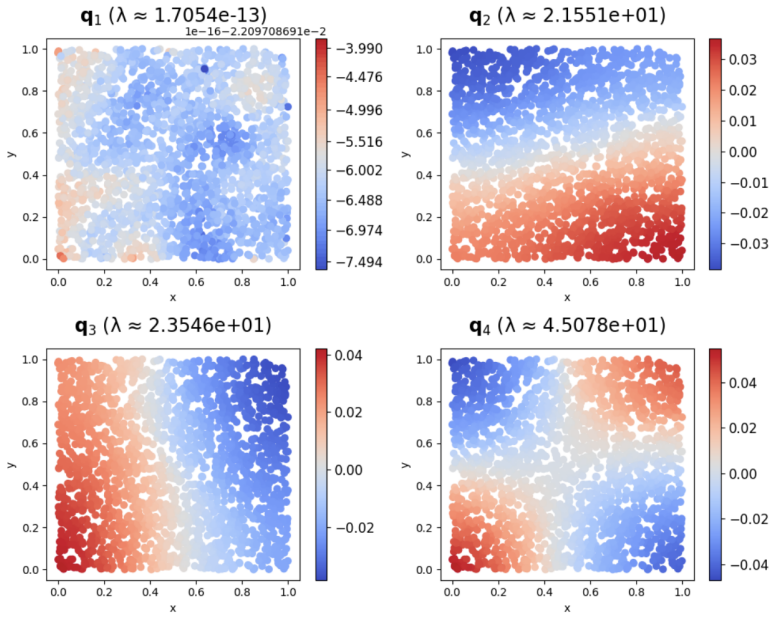

FIGURE 1. The First Four Smallest Eigenvectors of the Graph Laplacian for $m = 2048$

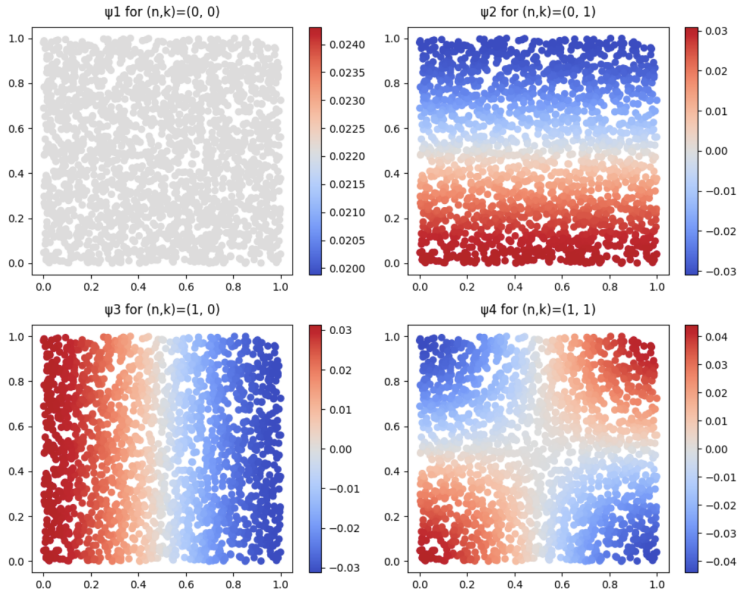

FIGURE 2. The First Eigenfunction of a Neumann Eigenvalue Problem for $m = 2048$

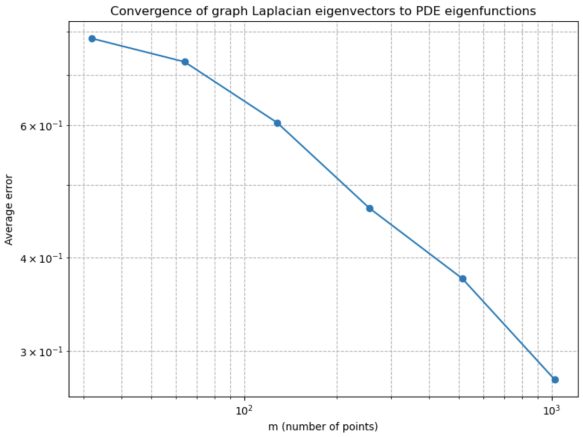

FIGURE 3. The Average Error between the Subspaces the Eigenvectors and Eigenfunction Span over 30 Trials for $m = \{2^7, 2^5, ..., 2^{10}\}$

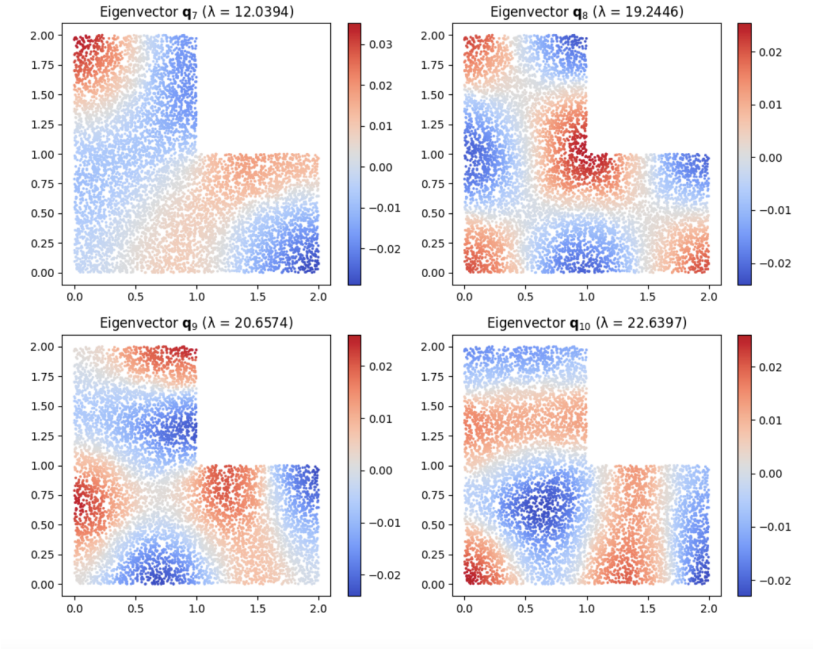

FIGURE 4. The First Four Smallest Eigenvectors for the Graph Laplacian on an L-shape domain for $m = 2^{13}$

4. Summary and Conclusions

In summary, the eigenvectors of a graph Laplacian L was implemented to approximate the eigenfunction of a Neumann eigenvalue problem on a unit box domain. The contour plot of the eigen entries in the box for the graph Laplacian shows color gradient consistency to the eigenfunction. The convergence of the eigenvectors to the discretized and normalized eigenfunction was by comparing the subspace each vector set span. The error decreases and the subspace of the eigenvector converges to the eigenfunction as the number of uniformly distributed points increase. In other words, for a sufficiently amount of scattered points, the graph Laplacian adequately approximates

the eigenfunction over a unit box. The graph Laplacian was further examined over an irregular L-shape domain. This leads to the question whether the eigenvectors of L suffice to approximate the eigenfunction over irregular boundaries as the analytical eigenfunction is hard to solve for.

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