AMATH 563: COMPARING THE GRAPH LAPLACIAN TO THE DIFFERENTIAL LAPLACE OPERATOR

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1. Introduction

In this report, we will construct a graph Laplacian operator that approximates the Laplacian differential operator. We initially defined a domain on the unit box. The eigenvectors from the differential operator and the eigenfunctions of the Laplacian operator were visualized on a contour plot, and the error was calculated between their projectors. We observed similar patterns within the contour plots between the two operators. In particular, we found that the first four eigenvectors of the graph Laplacian converge to the ones of the differential operator as we increase the number of points within our domain. We then consider an L-shaped domain and visualized the eigenvector values on a contour plot to observe oscillations in the eigenvector values across the domain.

2. Methods

2.1. **Part 1: Graph Laplacian.** First, we define our domain on the unit box with $\Omega = [0,1]^2 \subset \mathbb{R}$ where $X = x_1, \ldots, x_m$ are the set of uniformly distributed random points in Ω. We define the weighted graph $G = \{X, W\}$ where the weight matrix $W \in \mathbb{R}^{m \times m}$ is

$$w_{ij} = \kappa_\epsilon(\|\mathbf{x}_i - \mathbf{x}_j\|_2), \quad \text{with} \quad \kappa_\epsilon(t) := \begin{cases} (\pi\epsilon^2)^{-1} & t \leq \epsilon, \\ 0 & t > \epsilon. \end{cases}$$

The parameter $\epsilon > 0$ controls the bandwidth of the kernel κ which relates to the local connectivity of the graph G, and it is defined as

$$\epsilon(m) = C\frac{\log(m)^{3/4}}{m^{1/2}}$$

where for our purposes, we have the constant $C = 1$. We define the matrix

$$D = \mathrm{diag}(\mathbf{d}) \in \mathbb{R}^{m \times m}, \quad \mathbf{d} = W\mathbb{1}$$

where D is a diagonal matrix containing the sum along each row of W.

Let $L = D - W$ be our unnormalized graph Laplacian matrix of G. To compute the four smallest eigenvectors of L, defined as $\mathbf{q}_1, \ldots, \mathbf{q}_4 \in \mathbb{R}^m$, we use the `scipy.sparse` module and eigenvalue solver `eigsh`. Initially, we set $m = 2048$ to created a contour plot of the eigenvectors as functions over Ω.

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2.2. **Part 2: Differential Operator.** Now, consider the differential operator

$$\mathcal{L}f \mapsto -\left(\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2}\right),$$

that is well-defined for functions $f : \Omega \mapsto \mathbb{R}$, with $f \in C^2(\Omega)$. For integers $n, k \geq 0$, the functions

$$\psi(\mathbf{x}) = \cos(n\pi x_1)\cos(k\pi x_2),$$

solve the Neumann eigenvalue problem for the operator $\mathcal{L}$ such that

$$\begin{aligned} \mathcal{L}\psi &= \lambda(n,k)\psi, && \text{in } \Omega, \\ \nabla\psi \cdot \mathbf{n} &= 0, && \text{on Boundary of } \Omega. \end{aligned}$$

where $\mathbf{n}$ denotes the outward unit normal vector on the boundary of Ω.

We define the values for the first four eigenfunctions on X as $\tilde{\boldsymbol{\psi}}_j$ given the pairs $(n, k) \in \{(0, 0), (1, 0), (0, 1), (1, 1)\}$, such that we have the vectors $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_4 \in \mathbb{R}^m$,

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

Let $m = 2048$ where we then create a contour plot for the vectors $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_4$ over Ω.

2.3. **Part 3: Error.** Let $m = 2^4, 2^5, \ldots, 2^{10}$ and `n_trials` $= 30$. For each m and trial, we generate a random set X with $\epsilon(m)$ to compute the eigenvectors $\mathbf{q}_1, \ldots, \mathbf{q}_4$, along with the vectors $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_4$.

This is used to define the matrices

$$Q := [\mathbf{q}_1, \ldots, \mathbf{q}_4] \in \mathbb{R}^{m\times 4}, \qquad \Psi := [\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_4] \in \mathbb{R}^{m\times 4},$$

and the projectors

$$P_Q := QQ^T, \qquad P_\Psi := \Psi\Psi^T.$$

in order to compute the error,

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

The average error is then calculated for each m over all the trials, and then plotted in a loglog plot as a function of m.

2.4. **Part 4: L-shaped domain.** Let Ω be the L-shaped domain

$$\Omega = \left([0,1]^2\right) \cup ([1,2] \times [0,1]) \cup ([0,1] \times [1,2])$$

such that we add an additional square to the top and right of our original domain. Let $m = 2^{13}$ to generate uniformly random points X on Ω where we then plot the $\mathbf{q}_7, \ldots, \mathbf{q}_{10}$ eigenvectors of L on a contour plot.

3. Results

3.1. **Part 1: Graph Laplacian.** From calculating the first four eigenvectors of L, we see that our $\mathbf{q}_1$ is a constant eigenvector, corresponding to an eigenvalue $\lambda_1 = 0$ (Fig 1).

We observe that patterns start to emerge for the following eigenvectors, where the values of the second eigenvector $\mathbf{q}_2$ decreases in value as we move to the right in the domain Ω, while the values for $\mathbf{q}_3$ increases as we move down in Ω. This likely indicated a constant gradient in the value of the eigenvectors along one direction as we move across the domain. These two eigenvectors also have similar eigenvalues along the same order with $\lambda_2 \approx 0.2178$ and $\lambda_3 \approx 0.2401$.

As we move further up, we get $\lambda_4 \approx 0.43516$, almost double our previous eigenvalue. We observe an approximate saddle shape for the values of our eigenvalue $\mathbf{q}_4$, with high values along the top right and bottom left corners, and low values on the remaining corners.

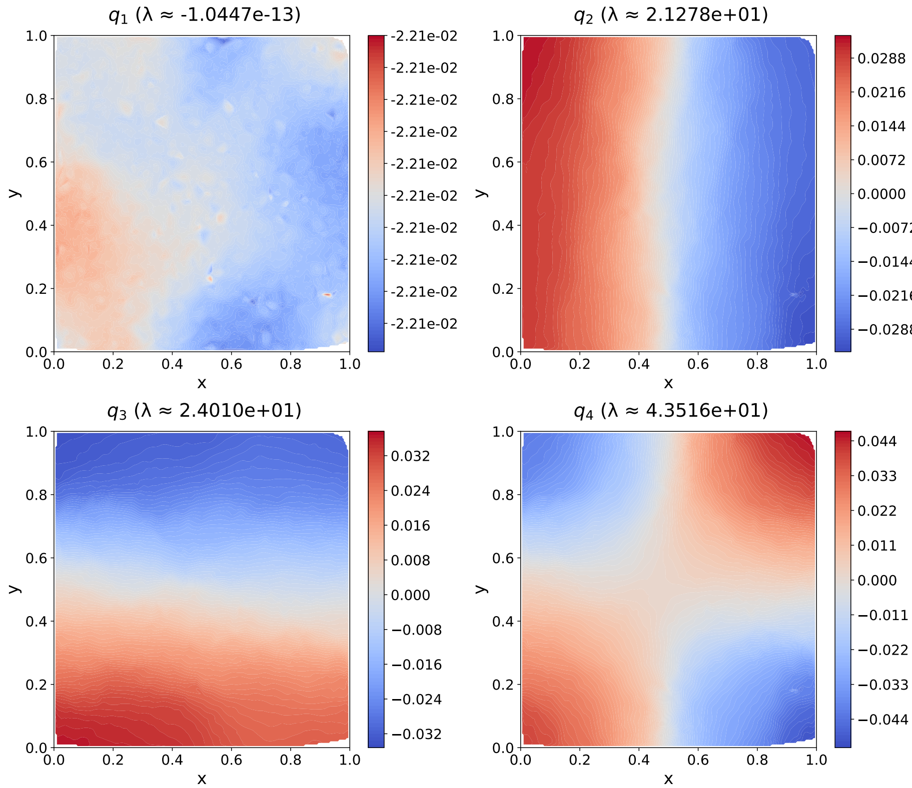

FIGURE 1. The first four eigenvectors of the graph Laplacian operator is plotted on the domain Ω given a uniformly random subset of points X, with the color bar indicating the value of the eigenvector at each point of the domain.

3.2. **Part 2: Differential Operator.** We observe similar patterns appear for $\boldsymbol{\psi}_i$ (Fig 2). This matches our eigenvector values closely, especially as we see the range of eigenvector values for each plot is within a similar range of values.

For the first eigenfunction $\boldsymbol{\psi}_1$, we have a constant value around 0.0221, which by a sign compared to $\mathbf{q}_1$, though this remains the same result as our eigenvalue here is 0. For $\boldsymbol{\psi}_2$ and $\boldsymbol{\psi}_3$, we observe a straighter and more uniform lines indicating the pattern and direction of the eigenvector. The maximum and minimum values between these two eigenfunctions are also closer together, indicating how close these two functions are.

3.3. **Part 3: Error.** We can quantify the difference between $\boldsymbol{\psi}_i$ and $\mathbf{q}_i$ by calculating and plotting the error between the projectors against m. From Figure 3, we see that as m increases, the error decreases, implying that q_i and ϕ_i will eventually converge as $m \to \infty$. The error remains in the same order of magnitude while m increases a few orders of magnitude, indicating a slow rate of convergence.

3.4. **Part 4: L-shaped domain.** Now consider our graph Laplacian on a different domain and their eigenvectors $\mathbf{q}_7, \ldots, \mathbf{q}_{10}$. We observe various patterns emerging on the domain (Fig 4).

For $\mathbf{q}_7$, we see that as we travel from the upper left to bottom right corner, the eigenvector value oscillates from low to high. Meanwhile, for $\mathbf{q}_8$, we get circular areas of highs and lows distributed across the domain, with the lower extrema in the center of the L, the top left, and the bottom right, while the higher extrema falls in between the pockets. With $\mathbf{q}_9$ and $\mathbf{q}_{10}$, we further observe oscillatory behavior, either from left to right or top to bottom, respectively.

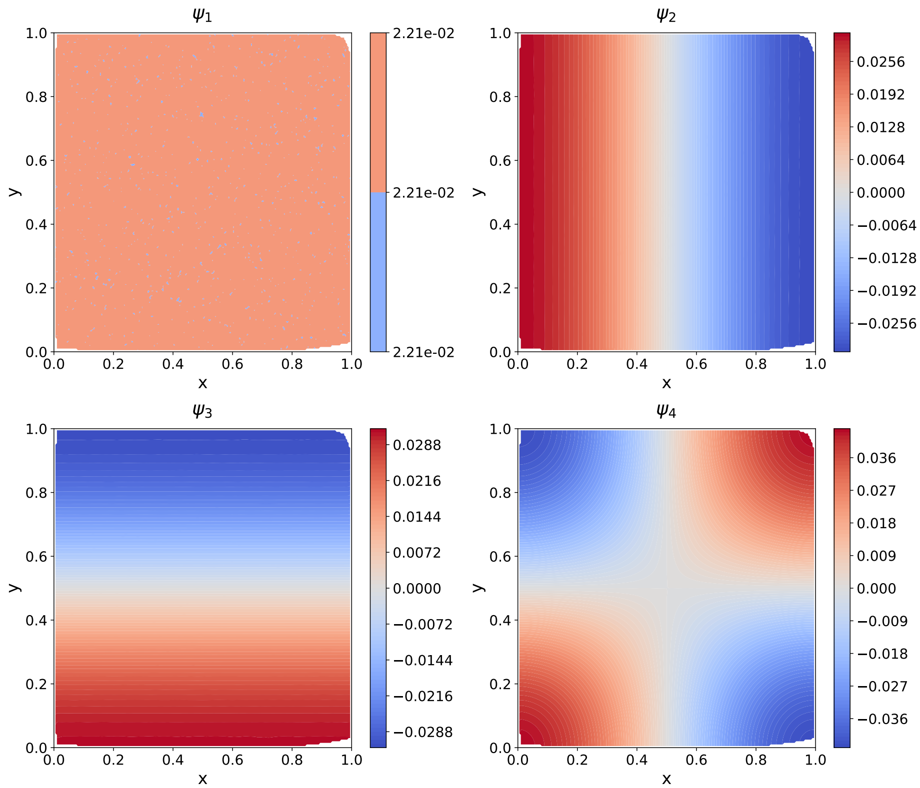

FIGURE 2. The first four eigenfunctions of the Laplacian operator is plotted on the domain Ω given a uniformly random subset of points X, with the color bar indicating the value of the eigenfunction at each point of the domain.

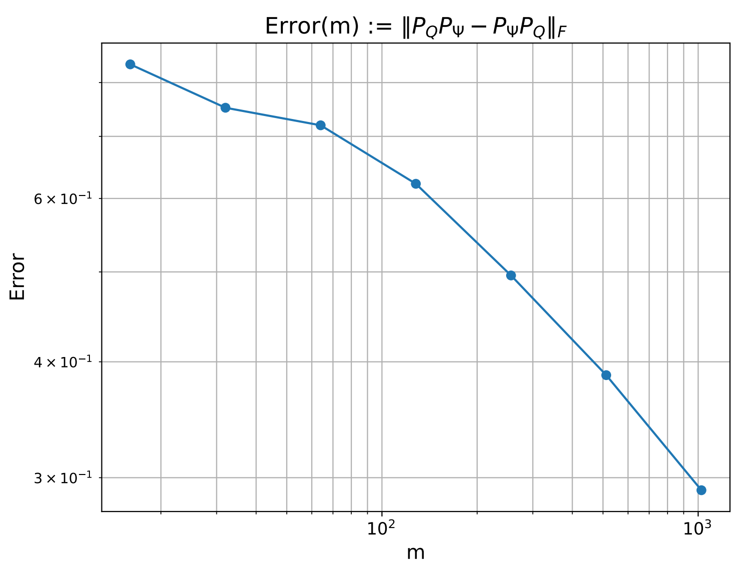

FIGURE 3. Error between the first four eigenvectors of the graph Laplacian and the first four eigenfunctions of the differential Laplace operator as m increases.

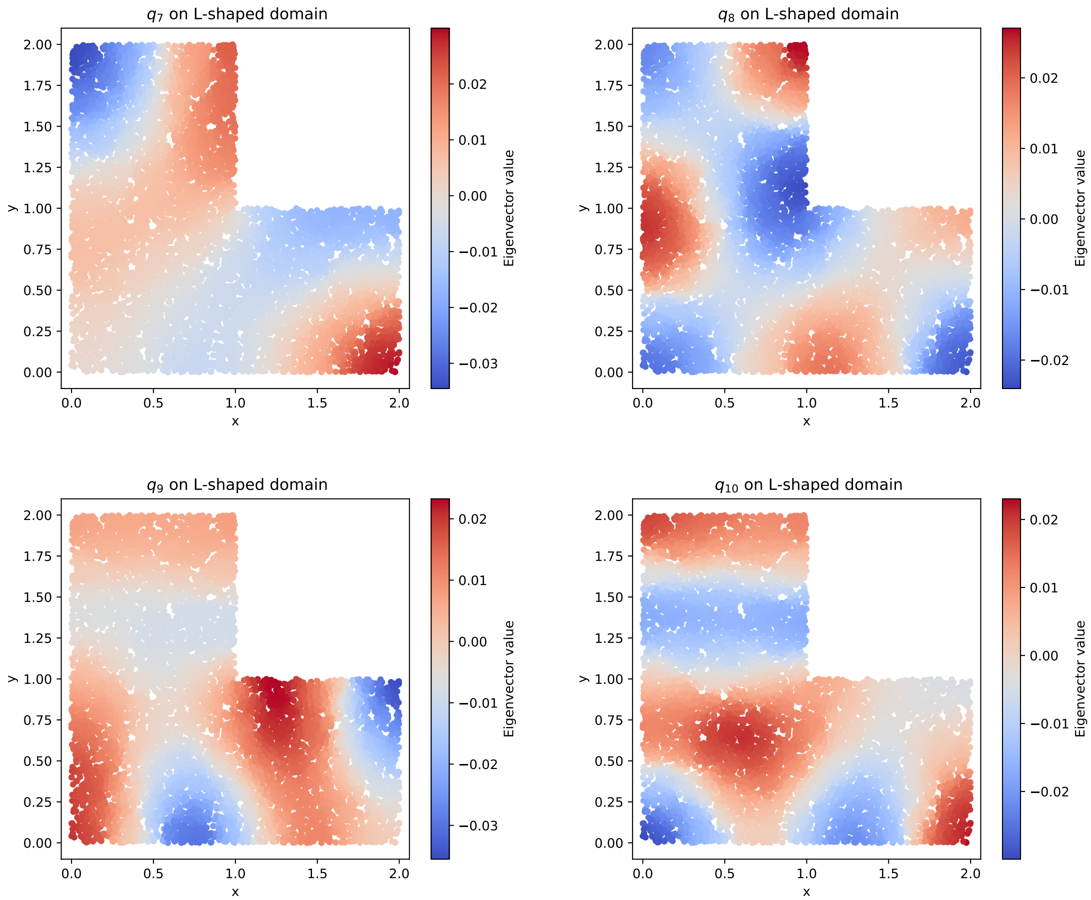

FIGURE 4. Contour plots for eigenvectors $\mathbf{q}_7, \ldots, \mathbf{q}_{10}$ of the graph Laplacian over the L-shaped domain.

4. Summary and Conclusions

From our plots and error calculations, we conclude that the spectrum of L converges slowly to that of $\mathcal{L}$ as $m \to \infty$. On the irregular shaped domain, we observed that the values of the eigenvectors $\mathbf{q}_7, \ldots, \mathbf{q}_{10}$ of the graph Laplacian oscillate across the domain between low and high values, which matches the definition of $\phi(x)$ which is a product of cosine functions on the domain.

Future directions to consider would be to consider other irregular domains to observe how the values of the eigenvectors change. Another direction is to alter the definition of the weight matrix and parameter C to explore how it affects the graph.

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