Homework 4

AMATH 563, Spring 2025

Due on May 26, 2025 at midnight.

Directions, Reminders and Policies

- You must upload two pdf files, one for theory questions and one for computational tasks to Gradescope.
- Make sure your solutions are well-written, complete, and readable for the theory question. I suggest you use Latex for your theory problems as well as your computational reports.
- For the computational tasks submit a pdf file typeset in Latex or any other typesetting software that can render equations appropriately. Please use the latex template provided on Canvas.
- I encourage collaborations and working with your colleagues to solve HW problems but you should only hand in your own work. We have a zero tolerance policy when it comes to academic misconduct and dishonesty including: Cheating; Falsification; Plagiarism; Engaging in prohibited behavior; Submitting the same work for separate courses without the permission of the instructor(s); Taking deliberate action to destroy or damage another person's academic work. **Such behavior will be reported to the UW Academic Misconduct office without warning**.

Theory Problems

1. Let $\mathcal{H}$ be an RKHS with kernel K and consider an optimization problem of the form

$$\min_{f \in \mathcal{H}} L(f(x_1), \dots, f(x_N)) + \frac{\lambda}{2}\|f\|_{\mathcal{H}}^2.$$

with $\lambda > 0$ and $L : \mathbb{R}^N \to \mathbb{R} \geq 0$.

   (a) Show that, if $K(X,X)$ is invertible, then every minimizer, if it exists, is of the form

$$f^\star(x) = K(x,X)K(X,X)^{-1}\mathbf{z}^\star$$

   where $\mathbf{z}^\star$ solves

$$\mathbf{z}^\star = \arg\min_{\mathbf{z}\in\mathbb{R}^N} L(z_1, \dots, z_N) + \frac{\lambda}{2}\mathbf{z}^T K(X,X)^{-1}\mathbf{z}.$$

   What do the entries of $\mathbf{z}^\star$ represent?

   (b) Further show that $f^\star$ can be equivalently written as

$$f^\star(x) = \sum_{i=1}^{N} z_i^\star \psi_i(x),$$

   where the $\psi_i \in \mathcal{H}$ are the functions defined by

$$\psi_i(x) = \arg\min_{\psi\in\mathcal{H}} \|\psi\|_{\mathcal{H}}^2 \quad \text{s.t.} \quad \psi_i(x_i) = 1, \quad \text{and} \quad \psi_i(x_j) = 0 \text{ for } j \neq i.$$

   (c) Finally show that the ψ_i are orthogonal to $\text{span}\{K(\cdot, x_j)\}_{j\neq i}$.

2. Let $L = D - W \in \mathbb{R}^{N\times N}$ be the unnormalized Laplacian and let $\tilde{L} = D^{-1/2}(D-W)D^{-1/2}$ be the normalized Laplacian. Show that

   (a) $(\lambda, \mathbf{v})$ is an eigenpair of $\tilde{L}$ iff $\mathbf{v} = D^{1/2}\mathbf{u}$ where $\mathbf{u}$ solves the generalized eigenvalue problem $L\mathbf{u} = \lambda D\mathbf{u}$.

   (b) Show that if G is a disconnected graph without isolated vertices and with M-connected components then $\tilde{L}$ has an M-dimensional null-space spanned by the weighted set functions $D^{1/2}\mathbf{1}_{G_j}$ where $\mathbf{1}_{G_j}$ is the indicator vector of the j-th connected component G_j.

   (c) Show that $\lambda_j \leq 2$ for all $j \leq n$, i.e., the eigenvalues of $\tilde{L}$ are uniformly bounded. Can you say the same about the eigenvalues of L? *Hint: Look up the Courant-Fisher-Weyl characterization of eigenvalues.*

Computational Problems

Solve the computational problem below. Perform the required tasks and hand in a report of a **maximum of six pages** *outlining your methodology, results, and findings. Use the computational report template provided on Canvas. You don't have to use Latex but it is highly recommended. Make sure that your figures and tables are readable, they are of good size, and labeled appropriately. Part of your grade will be assigned to the general tidiness and style of the report.* **You don't need to hand in your code.**

In this problem you will use a specific construction of the graph Laplacian operator to approximate the Laplacian differential operator on arbitrary domains. In parts 1–4 you work on the unit box and verify that the eigenvectors of the graph Laplacian converge to those of the differential operator. In part 5, you modify the domain to an L-shaped domain. In correspondence with the literature on graph Laplacians here we assume the eigenvalues of matrices are ordered in **increasing** order. *Some of the calculations here can be expensive and the matrices can become quite large. Make sure you take advantage of sparse matrices and benchmark your code with small data sets.*

1. Let $\Omega = [0,1]^2 \subset \mathbb{R}^2$ and let $x_1, \ldots, x_m$ be uniformly distributed random points in Ω. We define $X = \{x_1, \ldots, x_m\}$ to be our set of scattered data points and define the weighted graph $G = \{X, W\}$ with the weight matrix $W \in \mathbb{R}^{m \times m}$ as

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

The parameter $\varepsilon > 0$ controls the bandwidth of the kernel κ and in turn the local connectivity of the graph G. Throughout this assignment we choose

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

where $C > 0$ is a constant (you should find that $C = 1$ is sufficient but feel free to tune this number). Let $L = D - W$ be the unnormalized graph Laplacian matrix of G and fix $m = 2048$. Then compute the first four eigenvectors of L, i.e., those corresponding to the four smallest eigenvalues of L. Present a plot of these four eigenvectors as functions over Ω; you may use 3D scatter plots or contour plots.

2. 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 $f : \Omega \mapsto \mathbb{R}$ that are twice continuously differentiable, i.e., $f \in C^2(\Omega)$. Observe that for integers $n, k \ge 0$, the functions

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

solve the Neumann eigenvalue problem for the operator $\mathcal{L}$, i.e.,

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

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

Now let $\mathbf{q}_1, \ldots \mathbf{q}_4 \in \mathbb{R}^m$ be the eigenvectors of the graph Laplacian L as computed in part 1, and define the vectors $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_4 \in \mathbb{R}^m$ as follows

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

where the entries of $\tilde{\boldsymbol{\psi}}_j$ contain the point values of the first four eigenfunctions $\psi(x)$, at the vertices X. Once again fix $m = 2048$ and present a plot of the vectors $\boldsymbol{\psi}_1, \ldots \boldsymbol{\psi}_4$ akin to part 1. Inspect the plots visually and comment on similarities and differences between $\mathbf{q}_j$ and the $\boldsymbol{\psi}_j$.

3. We now wish to show that $\text{span}\{\mathbf{q}_1, \ldots, \mathbf{q}_4\} \approx \text{span}\{\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_4\}$. Choose $m = 2^7, 2^5, \ldots, 2^{10}$. For each value of m proceed as in part 1 to generate the random points X, compute the corresponding value

of $\varepsilon(m)$, and compute the four eigenvectors $\mathbf{q}_1, \dots, \mathbf{q}_4$. Also compute the vectors $\boldsymbol{\psi}_1, \dots, \boldsymbol{\psi}_4$ as above. Then define the matrices

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

and the projectors

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

Then compute the error

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

For each value of m, compute this error over at least 30 trials where the points in X are redrawn at random. Present a loglog plot of the average error as a function of m.

4. Hopefully the above results have convinced you that the spectrum of L converges to that of $\mathcal{L}$ as $m \to \infty$, albeit slowly. We now use this observation to approximate the spectrum of $\mathcal{L}$ on non-standard domains Ω. Let Ω be the L-shaped domain

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

i.e, the $[0,2]^2$ box with the top right quadrant removed. Take $m = 2^{13}$, generate uniformly random points X on Ω and proceed as in part 1 to plot the $\mathbf{q}_7, \dots, \mathbf{q}_{10}$ eigenvectors of L.