Homework 3

AMATH 563, Spring 2023

Due on May 12, 2023 at midnight.

Directions, Reminders and Policies

- You must upload a pdf file of your HW to Canvas by the due date.
- Make sure your solutions are well-written, complete, and readable.
- I suggest you use LaTeX(Overleaf is a great option) to prepare your HW and typeset your mathematical equations.
- If you prefer to hand in a handwritten solution then simply scan and upload the pdf.
- Remember you have two extension tokens that you can use for a day extension for your HWs throughout the quarter.
- 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**.

PROBLEMS

THEORY

1. Let $(\mathcal{H}, \|\cdot\|, \langle\cdot,\cdot\rangle)$ be an RKHS of functions from a set $\mathcal{X} \to \mathbb{R}$, with kernel K. Given a pointset $X = \{x_1, \dots, x_m\} \subset \mathcal{X}$ consider the interpolation problem

$$\begin{cases} \text{minimize}_{u \in \mathcal{H}} & \|u\| \\ \text{subject to} & u(X) = \mathbf{y}. \end{cases}$$

Suppose the x_m are distinct and that $K(X,X)$ is invertible. Prove that the minimizer $u^\star$ is given by the formula

$$u^\star = K(\cdot, X)K(X,X)^{-1}\mathbf{y}. \tag{1}$$

2. Let $(\mathcal{H}, \|\cdot\|, \langle\cdot,\cdot\rangle)$ be an RKHS of functions from a set $\mathcal{X} \to \mathbb{R}$, with kernel K.

   (a) Let $\phi \in \mathcal{H}^*$, be a bounded linear functional on $\mathcal{H}$. Show that the function $K\phi : x \mapsto \phi(K(\cdot, x))$ (this simply means the functional ϕ is applied to $K(\cdot, x)$ as a function from $\mathcal{X} \to \mathbb{R}$ for each fixed x) is the Riesz representer of ϕ with respect to the RKHS inner product. That is,

$$\phi(f) = \langle K\phi, f\rangle. \tag{2}$$

   Hint: (i) First consider the case of f belonging to the pre-Hilbert space $\mathcal{H}_0$; (ii) Observe that by taking ϕ to be the pointwise evaluation functional (2) is nothing more than the reproducing property.

   (b) Consider the setting of Problem 2. Let $\phi_1, \dots, \phi_m \in \mathcal{H}^*$ be a sequence of bounded linear functionals on $\mathcal{H}$. Show that the orthogonal complement of $\text{span}\{K\phi_1, \dots, K\phi_m\}$ is precisely the subspace

$$\{f \in \mathcal{H} \mid \phi_j(f) = 0, \quad j = 1, \dots, m\}.$$

   (c) Define the bounded linear operator

$$\boldsymbol{\phi} : \mathcal{H} \to \mathbb{R}^m, \qquad \boldsymbol{\phi}(f) := (\phi_1(f), \dots, \phi_m(f))^T,$$

   and consider the (generalized) interpolation problem

$$\begin{cases} \text{minimize}_{u \in \mathcal{H}} & \|u\| \\ \text{subject to} & \boldsymbol{\phi}(u) = \mathbf{y}. \end{cases}$$

   Consider the matrix $\Theta \in \mathbb{R}^{m \times m}$ with entries $\Theta_{ij} = \phi_i(K\phi_j)$. Prove that whenever Θ is invertible then the minimizer $u^\star$ is given by the formula

$$u^\star = \sum_{j=1}^m \alpha_j^\star K\phi_j, \qquad \text{where} \qquad \boldsymbol{\alpha}^\star = \Theta^{-1}.$$

   Hint: Observe that if the $\phi_j = \delta_{x_j}$ were pointwise evaluation functionals at a set of points $X = \{x_1, \dots, x_m\}$ then the above result coincides with formula (1).

3. 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 $\lambda_j \le 2$ for all $j \le n$, 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.*

Computation

Prepare a report of a maximum of four pages for this computational exercise addressing the tasks outlined below as well as pertinent mathematical background, algorithmic details, and your findings.

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 $x_1, \dots, x_m$ be uniformly distributed random points in Ω. We define $X = \{x_1, \dots, x_m\}$ 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 $\mathrm{span}\{\mathbf{q}_1, \ldots, \mathbf{q}_4\} \approx \mathrm{span}\{\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_4\}$. 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 $\mathbf{q}_1, \ldots, \mathbf{q}_4$. Also compute the vectors $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_4$ as above. Then 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

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

Then compute the error

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

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 $\mathbf{q}_7, \ldots, \mathbf{q}_{10}$ eigenvectors of L.