MAT 280: Harmonic Analysis on Graphs & Networks
Lecture 2: Prelude to Harmonic Analysis on Graphs — Laplacian Eigenfunctions on General Shape Domains

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Outline

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Introductory Comments

Hajime Urakawa (Emeritus Prof., Tohoku Univ.) said in 1999:

> *A long time ago, when I was a college student, I was told: "There is good mathematics around Laplacians." I engaged in mathematical research and education for a long time, but after all, I was just walking around "Laplacians," which appear in all sorts of places under different guises. When I reflect on the above proverb, however, I feel keenly that it represents an aspect of the important truth. I was ignorant at that time, but it turned out that "Laplacians" are one of the keywords to understand the vast field of modern mathematics.*

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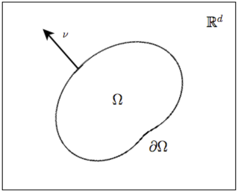
I second Prof. Urakawa's opinion, and want to add: *"There are good applications around Laplacians too."*

Outline

Motivations

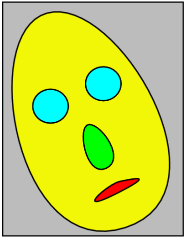
- Consider a bounded domain of general shape $\Omega \subset \mathbb{R}^d$.
- Want to analyze the spatial frequency information *inside* of the object defined in $\Omega \Longrightarrow$ need to avoid *the Gibbs phenomenon* due to $\partial\Omega$.
- Want to *represent* the object information efficiently for analysis, interpretation, discrimination, etc. $\Longrightarrow$ need *fast decaying* expansion coefficients relative to a *meaningful* basis.
- Want to extract and analyze *geometric information* about the domain $\Omega \Longrightarrow$ M. Kac: *"Can one hear the shape of a drum?"* (1966); spectral geometry; shape clustering/classification.



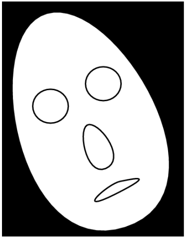
(a) $\Omega \subset \mathbb{R}^d$

(b) M. Kac (1914–1984)

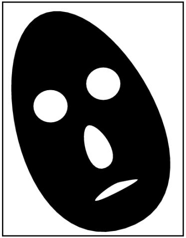
Object-Oriented Image Analysis



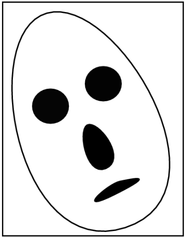
(a) Original



(b) Background

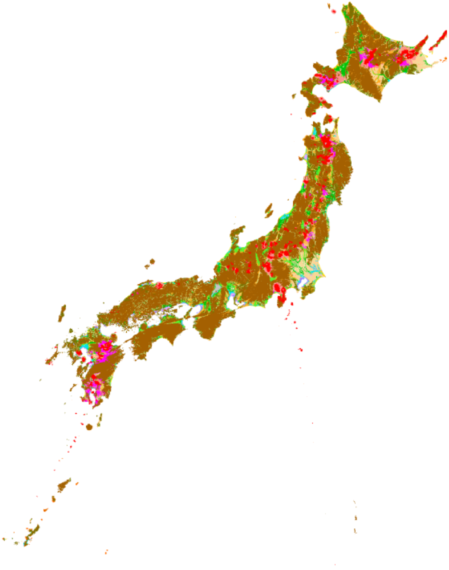


(c) Object

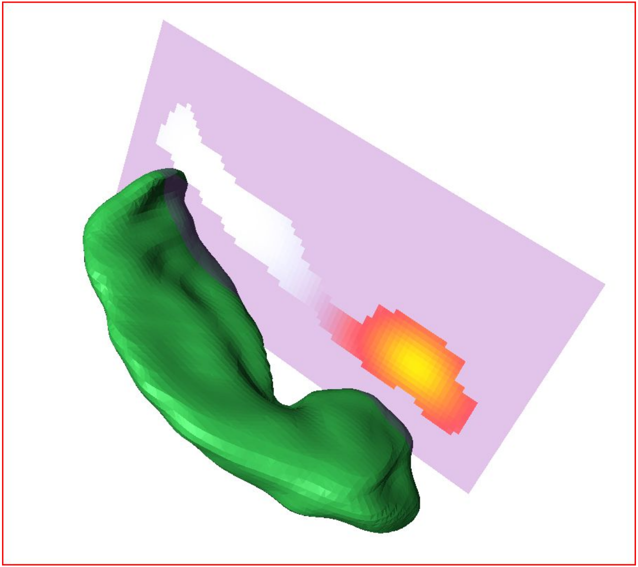


(d) Anomalies

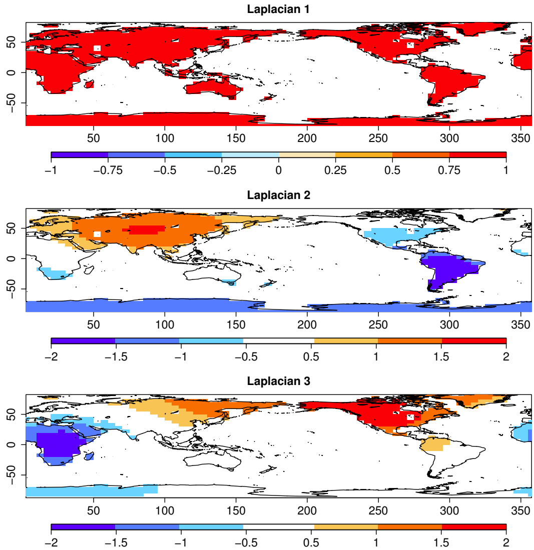
Data Analysis on a Complicated Domain



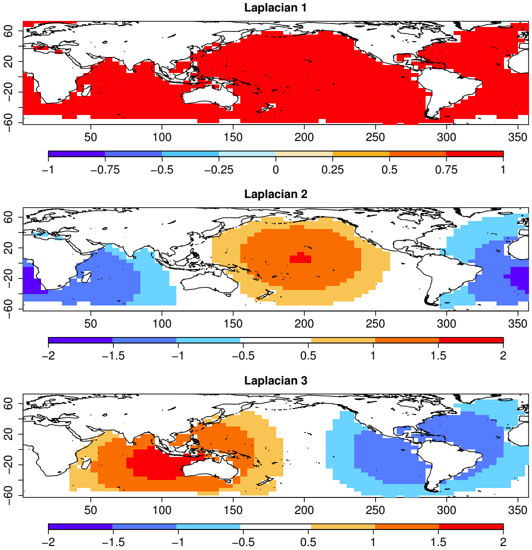
3D Hippocampus Shape Analysis (Courtesy: F. Beg)



Climate Data Analysis: Continent (Courtesy: T. DelSole)



Climate Data Analysis: Ocean (Courtesy: T. DelSole)



Outline

Enter Laplacian Eigenfunctions!

- On either irregular Euclidean domains or graphs, appropriately defined *Laplacian eigenfunctions* play an important role for data analysis.
- Let us first consider an irregular (i.e., general shape) Euclidean domain $\Omega \subset \mathbb{R}^d$.
- Let $\mathscr{L} := -\Delta = -\left(\frac{\partial^2}{\partial {x_1}^2} + \cdots + \frac{\partial^2}{\partial {x_d}^2}\right)$.
- The Laplacian eigenvalue problem is defined as:

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

  together with some appropriate boundary condition (BC).
- Most common (homogeneous) BCs are:
  - *Dirichlet:* $u = 0$ on $\partial\Omega$;
  - *Neumann:* $\frac{\partial u}{\partial \nu} = 0$ on $\partial\Omega$;
  - *Robin (or impedance):* $au + b\frac{\partial u}{\partial \nu} = 0$ on $\partial\Omega$, $a \neq 0 \neq b$.

Laplacian Eigenfunctions . . . Why?

- Why not analyze (and synthesize) an object of interest defined or measured on an irregular domain Ω using *genuine basis functions tailored to the domain* instead of the basis functions developed for rectangles, tori, balls, etc.?
- After all, *sines* (and *cosines*) are the eigenfunctions of the Laplacian on a *rectangular* domain (e.g., an interval in 1D) with Dirichlet (and Neumann) boundary condition.
- *Spherical harmonics, Bessel functions, and Prolate Spheroidal Wave Functions*, are part of the eigenfunctions of the Laplacian (via separation of variables) for the *spherical, cylindrical, and spheroidal* domains, respectively.
- Laplacian eigenfunctions (LEs) allow us to perform *spectral analysis* of data measured at more general domains or even on *graphs* and *networks* $\Longrightarrow$ *Generalization of Fourier analysis!*
- The above statement needs to be interpreted very carefully due to the domain properties; e.g., quantum scars, LE localizations, . . .
  $\Longrightarrow$ We will discuss more when we cover *wavelets on graphs*.

Laplacian Eigenfunctions ... Some Facts & Difficulties

- Analysis of $\mathscr{L}$ is difficult due to its *unboundedness* (because it is a *differential operator* dealing with *local* information).
- Much better to analyze its inverse, i.e., the *Green's operator*, because it is an *integral operator* dealing with *global* information, i.e., it's *compact* and *self-adjoint*.
- Thus $\mathscr{L}^{-1}$ has discrete spectra (i.e., a countable number of eigenvalues with finite multiplicity) except 0 spectrum.
- $\mathscr{L}$ has a complete orthonormal basis of $L^2(\Omega)$, and this allows us to do *eigenfunction expansion* in $L^2(\Omega)$.
- The key difficulty is to compute such eigenfunctions; directly solving the Helmholtz equation (or eigenvalue problem) on a general domain is tough.
- Unfortunately, computing the Green's function for a general Ω satisfying the usual boundary condition (i.e., Dirichlet, Neumann, Robin) is also very difficult.

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Integral Operators Commuting with Laplacian

- The key idea to avoid difficulties associated with the Laplacian $\mathscr{L}$ is to find an integral operator $\mathscr{K}$ *commuting* with $\mathscr{L}$ without imposing the strict boundary condition a priori.
- Then, we know that the eigenfunctions of $\mathscr{L}$ is the same as those of $\mathscr{K}$, which is easier to deal with, due to the following

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Theorem (G. Frobenius 1896?; B. Friedman 1956)

Suppose $\mathscr{K}$ and $\mathscr{L}$ commute and one of them has an eigenvalue with finite multiplicity. Then, $\mathscr{K}$ and $\mathscr{L}$ share the same eigenfunction corresponding to that eigenvalue. That is, $\mathscr{L}\varphi = \lambda\varphi$ and $\mathscr{K}\varphi = \mu\varphi$.

(a) G. Frobenius (1849–1917)

(b) B. Friedman (1915–1966)

- The inverse of $\mathscr{L}$ with some specific boundary condition (e.g., Dirichlet/Neumann/Robin) is also an integral operator whose kernel is called the *Green's function* $G(\boldsymbol{x},\boldsymbol{y})$.
- Since it is not easy to obtain $G(\boldsymbol{x},\boldsymbol{y})$ in general, let's replace $G(\boldsymbol{x},\boldsymbol{y})$ by the *fundamental solution of the Laplacian*:

$$K(\boldsymbol{x},\boldsymbol{y}) = \begin{cases} -\frac{1}{2}|x-y| & \text{if } d=1, \\ -\frac{1}{2\pi}\log|\boldsymbol{x}-\boldsymbol{y}| & \text{if } d=2, \\ \frac{|\boldsymbol{x}-\boldsymbol{y}|^{2-d}}{(d-2)\omega_d} & \text{if } d>2, \end{cases}$$

where $\omega_d := \frac{2\pi^{d/2}}{\Gamma(d/2)}$ is the surface area of the unit ball in $\mathbb{R}^d$, and $|\cdot|$ is the standard Euclidean norm.

- The price we pay is to have rather implicit, *non-local* boundary condition although we do not have to deal with this condition directly.

- Let $\mathscr{K}$ be the integral operator with its kernel $K(\boldsymbol{x}, \boldsymbol{y})$:

$$\mathscr{K} f(\boldsymbol{x}) := \int_{\Omega} K(\boldsymbol{x}, \boldsymbol{y}) f(\boldsymbol{y}) \,\mathrm{d}\boldsymbol{y}, \quad f \in L^2(\Omega).$$

Theorem (NS 2005, 2008)

The integral operator $\mathscr{K}$ commutes with the Laplacian $\mathscr{L} = -\Delta$ with the following non-local boundary condition:

$$\int_{\partial\Omega} K(\boldsymbol{x}, \boldsymbol{y}) \frac{\partial \varphi}{\partial \nu_{\boldsymbol{y}}}(\boldsymbol{y}) \,\mathrm{d}s(\boldsymbol{y}) = -\frac{1}{2}\varphi(\boldsymbol{x}) + \mathrm{pv}\int_{\partial\Omega} \frac{\partial K(\boldsymbol{x}, \boldsymbol{y})}{\partial \nu_{\boldsymbol{y}}} \varphi(\boldsymbol{y}) \,\mathrm{d}s(\boldsymbol{y}), \quad \forall \boldsymbol{x} \in \partial\Omega,$$

where φ is an eigenfunction common for both operators, and pv indicates the Cauchy principal value.

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Corollary (NS 2009)

The eigenfunction $\varphi(\boldsymbol{x})$ of the integral operator $\mathscr{K}$ in the previous theorem can be extended outside the domain Ω and satisfies the following equation:

$$-\Delta\varphi = \begin{cases} \lambda\varphi & \text{if } \boldsymbol{x} \in \Omega; \\ 0 & \text{if } \boldsymbol{x} \in \mathbb{R}^d \setminus \overline{\Omega}, \end{cases}$$

with the boundary condition that φ and $\dfrac{\partial\varphi}{\partial\nu}$ are continuous across the boundary $\partial\Omega$. Moreover, as $|\boldsymbol{x}| \to \infty$, $\varphi(\boldsymbol{x})$ must be of the following form:

$$\varphi(\boldsymbol{x}) = \begin{cases} \text{const} \cdot |\boldsymbol{x}|^{2-d} + O\left(|\boldsymbol{x}|^{1-d}\right) & \text{if } d \neq 2; \\ \text{const} \cdot \ln|\boldsymbol{x}| + O\left(|\boldsymbol{x}|^{-1}\right) & \text{if } d = 2. \end{cases}$$

Corollary (NS 2005, 2008)

The integral operator $\mathscr{K}$ *is compact and self-adjoint on* $L^2(\Omega)$*. Thus, the kernel* $K(\boldsymbol{x}, \boldsymbol{y})$ *has the following* eigenfunction expansion *(in the sense of mean convergence):*

$$K(\boldsymbol{x}, \boldsymbol{y}) \sim \sum_{j=1}^{\infty} \mu_j \varphi_j(\boldsymbol{x}) \overline{\varphi_j(\boldsymbol{y})},$$

and $\{\varphi_j\}_j$ *forms an orthonormal basis of* $L^2(\Omega)$*.*

Outline

1D Example

- Consider the unit interval $\Omega = (0, 1)$.
- Then, our integral operator $\mathscr{K}$ with the kernel $K(x, y) = -|x - y|/2$ gives rise to the following eigenvalue problem:

$$-\varphi'' = \lambda\varphi, \quad x \in (0, 1);$$

$$\varphi(0) + \varphi(1) = -\varphi'(0) = \varphi'(1).$$

- The kernel $K(\boldsymbol{x}, \boldsymbol{y})$ is of *Toeplitz* form $\Longrightarrow$ Eigenvectors must have even and odd symmetry (Cantoni-Butler '76).
- In this case, we have the following explicit solution.

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- $\lambda_0 \approx -5.756915$, which is a solution of $\tanh \frac{\sqrt{-\lambda_0}}{2} = \frac{2}{\sqrt{-\lambda_0}}$,

$$\varphi_0(x) = A_0 \cosh \sqrt{-\lambda_0}\left(x - \frac{1}{2}\right);$$

- $\lambda_{2m-1} = (2m-1)^2\pi^2,\ m = 1, 2, \ldots,$

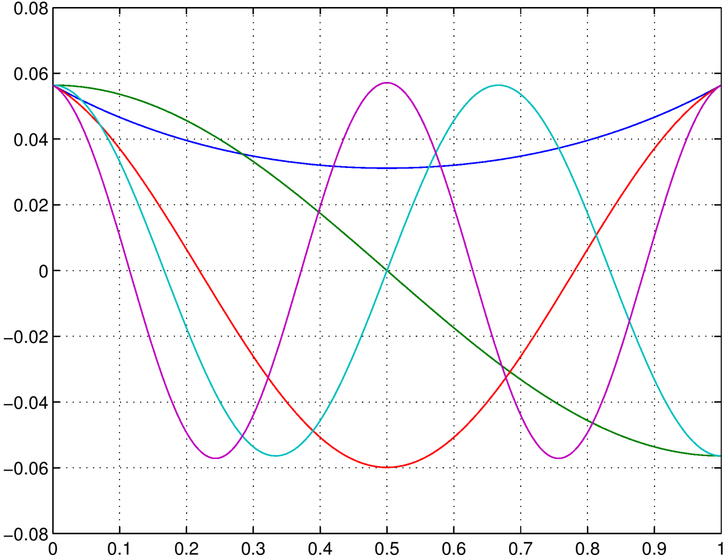
$$\varphi_{2m-1}(x) = \sqrt{2}\cos(2m-1)\pi x;$$

- $\lambda_{2m},\ m = 1, 2, \ldots,$ which are solutions of $\tan \frac{\sqrt{\lambda_{2m}}}{2} = -\frac{2}{\sqrt{\lambda_{2m}}}$,

$$\varphi_{2m}(x) = A_{2m} \cos \sqrt{\lambda_{2m}}\left(x - \frac{1}{2}\right),$$

where $A_k,\ k = 0, 1, \ldots$ are normalization constants.

First 5 Basis Functions



1D Example: Comparison

- The Laplacian eigenfunctions with the Dirichlet boundary condition: $-\varphi'' = \lambda\varphi$, $\varphi(0) = \varphi(1) = 0$, are *sines*. The Green's function in this case is:

$$G_D(x, y) = \min(x, y) - xy.$$

- Those with the Neumann boundary condition, i.e., $\varphi'(0) = \varphi'(1) = 0$, are *cosines*. The Green's function is:

$$G_N(x, y) = -\max(x, y) + \frac{1}{2}(x^2 + y^2) + \frac{1}{3}.$$

- Remark: Gridpoint ⇔ DST-I/DCT-I;
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2D Example

- Consider the unit disk Ω. Then, our integral operator $\mathscr{K}$ with the kernel $K(\boldsymbol{x},\boldsymbol{y}) = -\frac{1}{2\pi}\log|\boldsymbol{x}-\boldsymbol{y}|$ gives rise to:

$$-\Delta\varphi = \lambda\varphi, \quad \text{in } \Omega;$$

$$\left.\frac{\partial\varphi}{\partial\nu}\right|_{\partial\Omega} = \left.\frac{\partial\varphi}{\partial r}\right|_{\partial\Omega} = -\left.\frac{\partial\mathscr{H}\varphi}{\partial\theta}\right|_{\partial\Omega},$$

where $\mathscr{H}$ is the *Hilbert transform* for the circle, i.e.,

$$\mathscr{H}f(\theta) := \frac{1}{2\pi}\,\mathrm{pv}\!\int_{-\pi}^{\pi} f(\eta)\cot\left(\frac{\theta-\eta}{2}\right)\mathrm{d}\eta \quad \theta\in[-\pi,\pi].$$

- Let $j_{k,\ell}$ is the ℓth zero of the Bessel function of order k, $J_k(j_{k,\ell})=0$. Then,

$$\varphi_{m,n}(r,\theta) = \begin{cases} J_m(j_{m-1,n}\,r)\binom{\cos}{\sin}(m\theta) & \text{if } m=1,2,\ldots,\ n=1,2,\ldots, \\ J_0(j_{0,n}\,r) & \text{if } m=0,\ n=1,2,\ldots, \end{cases}$$

$$\lambda_{m,n} = \begin{cases} j_{m-1,n}^2, & \text{if } m=1,\ldots,\ n=1,2,\ldots, \\ j_{0,n}^2 & \text{if } m=0,\ n=1,2,\ldots. \end{cases}$$

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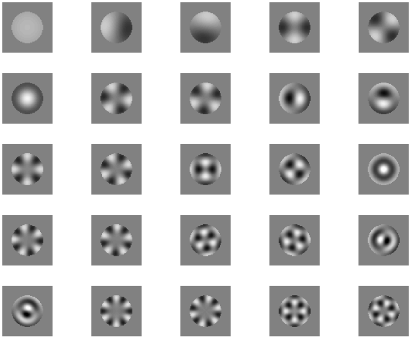
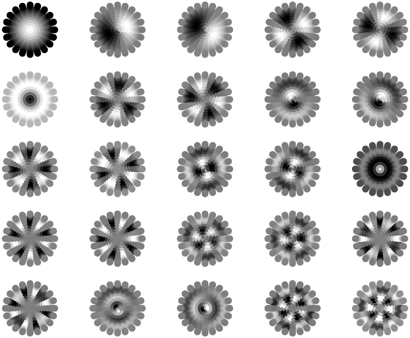
First 25 Basis Functions



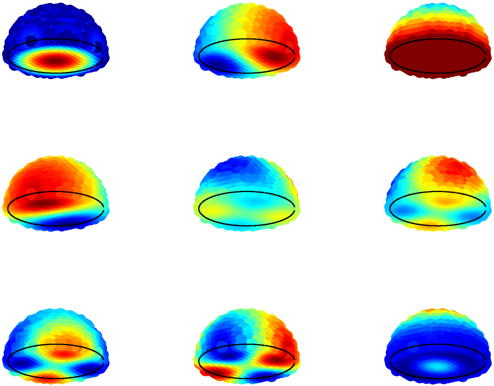
(a) Our Basis



(b) Dirichlet-Laplace

3D Example

- Consider the unit ball Ω in $\mathbb{R}^3$. Then, our integral operator $\mathscr{K}$ with the kernel $K(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}$.
- Top 9 eigenfunctions cut at the equator viewed from the south:



Outline

Discretization of the Problem

- Assume that the whole dataset consists of a collection of data sampled on a regular grid, and that each sampling cell is a box of size $\prod_{i=1}^{d} \Delta x_i$.
- Assume that an object of our interest Ω consists of a subset of these boxes whose centers are $\{\boldsymbol{x}_i\}_{i=1}^{N}$.
- Under these assumptions, we can approximate the integral eigenvalue problem $\mathscr{K}\varphi = \mu\varphi$ with a simple quadrature rule with node-weight pairs $(\boldsymbol{x}_j, w_j)$ as follows.

$$\sum_{j=1}^{N} w_j K(\boldsymbol{x}_i, \boldsymbol{x}_j)\varphi(\boldsymbol{x}_j) = \mu\varphi(\boldsymbol{x}_i), \quad i = 1, \ldots, N, \quad w_j = \prod_{i=1}^{d} \Delta x_i.$$

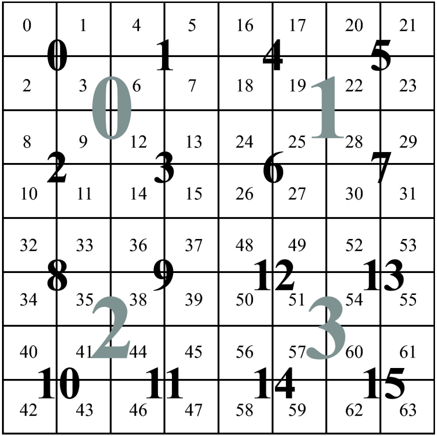
- Let $K_{i,j} := w_j K(\boldsymbol{x}_i, \boldsymbol{x}_j)$, $\varphi_i := \varphi(\boldsymbol{x}_i)$, and $\boldsymbol{\varphi} := (\varphi_1, \ldots, \varphi_N)^{\mathsf{T}} \in \mathbb{R}^N$. Then, the above equation can be written in a matrix-vector format as: $K\boldsymbol{\varphi} = \mu\boldsymbol{\varphi}$, where $K = (K_{ij}) \in \mathbb{R}^{N \times N}$. Under our assumptions, the weight w_j does not depend on j, which makes K *symmetric*.

Outline

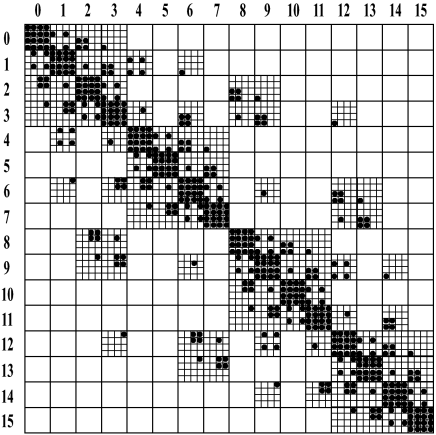
A Possible Fast Algorithm for Computing φ_j's

- Observation: our kernel function $K(\boldsymbol{x}, \boldsymbol{y})$ is of special form, i.e., the fundamental solution of Laplacian used in *potential theory*.
- Idea: Accelerate the matrix-vector product $K\boldsymbol{\varphi}$ using the *Fast Multipole Method* (FMM).
- Convert the kernel matrix to the tree-structured matrix via the FMM whose submatrices are nicely organized in terms of their *ranks*. (Computational cost: our current implementation costs $O(N^2)$, but can achieve $O(N \log N)$ via the randomized SVD algorithm of Woolfe-Liberty-Rokhlin-Tygert (2008)).
- Construct $O(N)$ matrix-vector product module fully utilizing rank information (See also the work of Bremer (2007) and the "HSS" algorithm of Chandrasekaran et al. (2006)).
- Embed that matrix-vector product module in the Krylov subspace method, e.g., Lanczos iteration.
  (Computational cost: $O(N)$ for each eigenvalue/eigenvector).

Tree-Structured Matrix via FMM

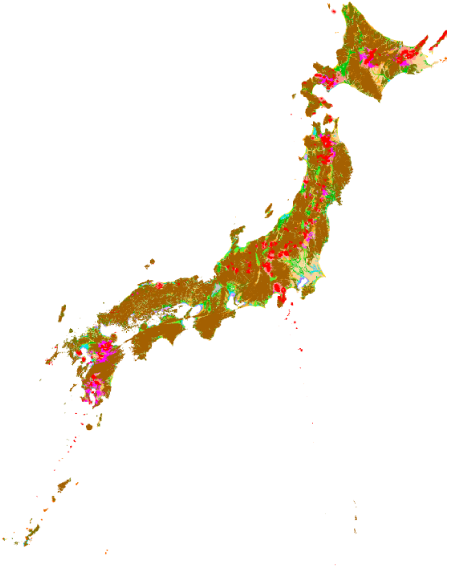


(a) Hierarchical indexing scheme

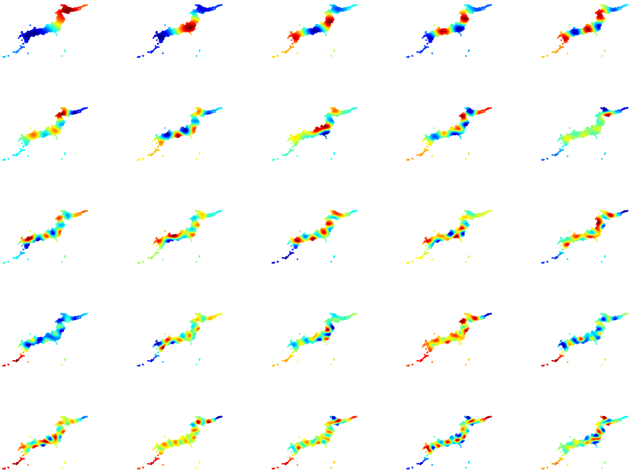


(b) Tree-Structured Matrix

A Real Challenge: Kernel matrix is of 387924×387924.



First 25 Basis Functions via the FMM-based algorithm



Outline

General Comments on Applications

Laplacian eigenfunctions on an irregular domain should be useful for:

- Interactive image analysis, discrimination, interpretation:
  - Medical image analysis: e.g., hippocampal shape analysis for early Alzheimer's
  - Biometry: e.g., identification and characterization of eyes, faces, etc.
- Geophysical data assimilation:
  - Incorporating ocean current data measured by high frequency radar into a numerical model;
  - Interpolation, extrapolation, prediction of vector-valued meteorology data (temperature, pressure, wind speed, etc.) measured at the weather station in the 3D terrain.
- ...

Due to the time constraint, I will only talk about one application.

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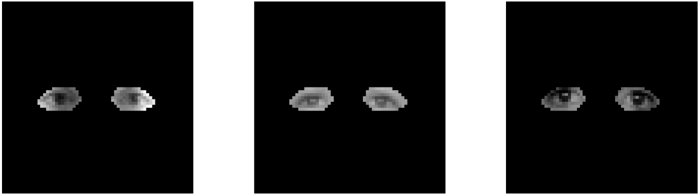
Statistical Image Analysis; Comparison with PCA

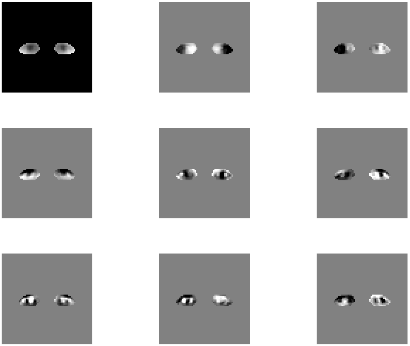
- Consider a stochastic process living on a domain Ω.
- *PCA/Karhunen-Loève Transform* is often used.
- PCA/KLT *implicitly* incorporate geometric information of the measurement (or pixel) location through *data correlation*.
- Our Laplacian eigenfunctions use *explicit* geometric information through the harmonic kernel $K(\boldsymbol{x}, \boldsymbol{y})$.

Comparison with PCA: Example

- *"Rogue's Gallery"* dataset from Larry Sirovich
- Contains 143 faces
- Extracted left & right eye regions

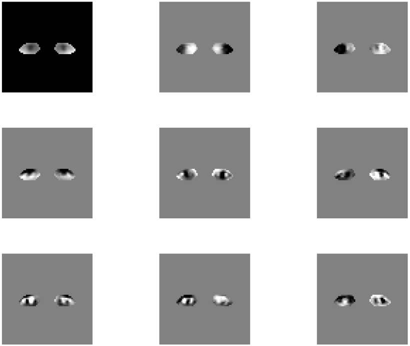


Comparison with PCA: Basis Vectors

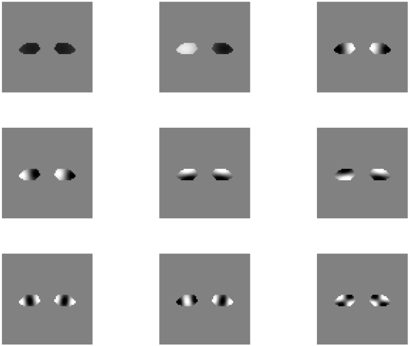


(a) KLB/PCA 1:9

Comparison with PCA: Basis Vectors

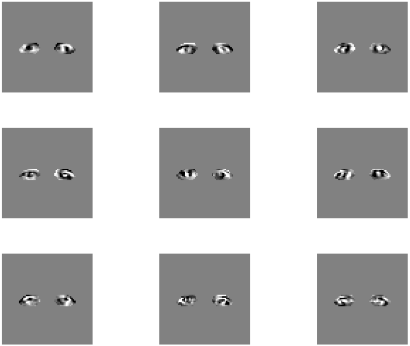


(a) KLB/PCA 1:9

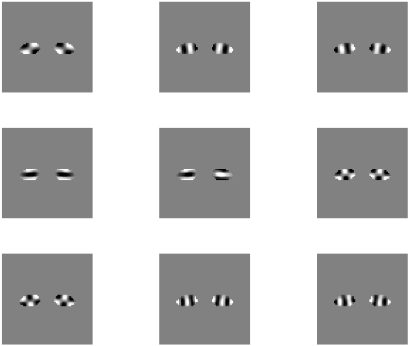


(b) Laplacian Eigenfunctions 1:9

Comparison with PCA: Basis Vectors . . .

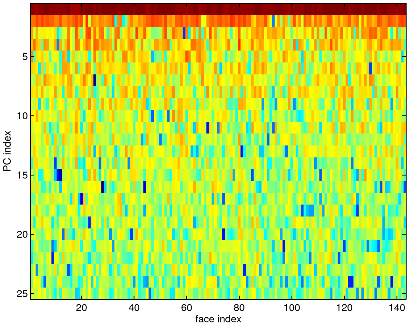


(a) KLB/PCA 10:18

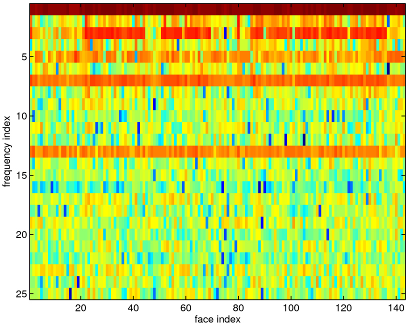


(b) Laplacian Eigenfunctions 10:18

Comparison with PCA: Energy Distribution over Coordinates

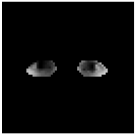


(a) KLB/PCA

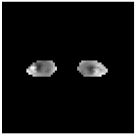


(b) Laplacian Eigenfunctions

Comparison with PCA: Basis Vector #7 . . .

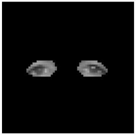


c_7:large

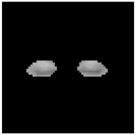


c_7:large

φ_7

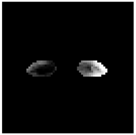


c_7:small

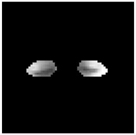


c_7:small

Comparison with PCA: Basis Vector #13 . . .



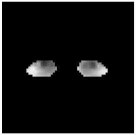
c_{13}:large



c_{13}:large

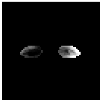
φ_{13}

c_{13}:small

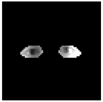


c_{13}:small

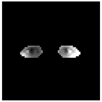
Asymmetry Detector



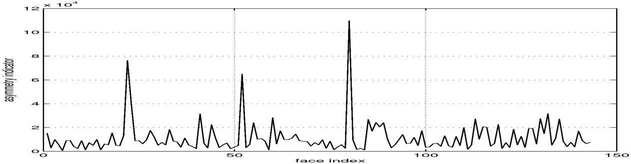
Eyes #80



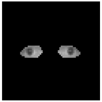
Eyes #22



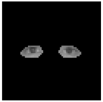
Eyes #52



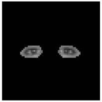
Asymmetry detector



Eyes #5



Eyes #84



Eyes #59

Outline

Summary

Our approach using the commuting integral operators

- Allows *object-oriented* signal/image analysis & synthesis
- Can get fast-decaying expansion coefficients (less Gibbs effect)
- Can naturally extend the basis functions outside of the initial domain
- Can extract *geometric information* of a domain through eigenvalues
- Can *decouple* geometry/domain information and statistics of data
- Is closely related to the *von Neumann-Kreĭn Laplacian*, yet is distinct
- Can use *Fast Multipole Methods* to speed up the computation, which is the key for higher dimensions/large domains

Future Plan (i.e., PhD Research Topics)

$\exists$ many things to do:

- Examine further our boundary conditions for specific geometry in higher dimensions; e.g., analysis on $\mathbb{S}^2$ leads to *Clifford Analysis*
- Examine the relationship with the *von Neuman-Kreĭn Laplacian* and *Volterra operators* in $\mathbb{R}^d$, $d \geq 2$ (Lidskiĭ; Gohberg-Kreĭn)
- Examine integral operators commuting with *polyharmonic* operators $(-\Delta)^p$, $p \geq 2$
- Extend integral operators to the *manifold* setting (e.g., on *curved* surfaces) $\Longrightarrow$ Need to consider *geodesic distance between a pair of points*
- Extend integral operators to the *graph* setting $\Longrightarrow$ Need to consider *shortest distance between a pair of nodes* and a function of the *distance matrix* instead of *graph Laplacian*

My Heroes

(a) George Green (1793–1841)

(b) Lord Rayleigh (1842–1919)

(c) H.K.H. Weyl (1885–1955)

(d) J. von Neumann (1903–1957)

(e) Mark G. Kreĭn (1907–1989)

(f) M. Kac (1914–1984)

(g) V. Lidskiĭ (1924–2008)

(h) I. Gohberg (1928–2009)

(i) V. Rokhlin (1952–)

(j) L. Greengard (1958–)

References

- Laplacian Eigenfunction Resource Page
  http://www.math.ucdavis.edu/~saito/lapeig/:
  - My Course Note (elementary) on "Laplacian Eigenfunctions: Theory, Applications, and Computations"
  - All the talk slides of the minisymposia on Laplacian Eigenfunctions at: ICIAM 2007, Zürich; SIAM Imaging Science Conference 2008, San Diego; IPAM 2009; SIAM Annual Meeting 2013, San Diego; and the other related recent minisymposia.
- The following articles are available at
  http://www.math.ucdavis.edu/~saito/publications/:

  - N. Saito: "Data analysis and representation using eigenfunctions of Laplacian on a general domain," *Applied & Computational Harmonic Analysis*, vol. 25, no. 1, pp. 68–97, 2008.
  - L. Hermi & N. Saito: "On Rayleigh-type formulas for a non-local boundary value problem associated with an integral operator commuting with the Laplacian," *Applied & Computational Harmonic Analysis*, vol. 45, no. 1, pp. 59–83. 2018.