

MAT 207B Lectures 26, 27, 28

Laplacian Eigenfunctions: Foundations and Applications

Naoki Saito

Department of Mathematics
University of California, Davis

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Outline

- 1 Motivations
- 2 History of Laplacian Eigenvalue Problems – Spectral Geometry
- 3 Harmonic Analysis of/on Irregular Domains via Eigenfunctions of Integral Operators Commuting with Laplacians
- 4 Summary & References

Acknowledgment

- Mark Ashbaugh (Univ. Missouri)
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- My current & former students at UC Davis
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- The MacTutor History of Mathematics Archive, Wikipedia, . . .

General Basic References

- W. A. Strauss: *Partial Differential Equations: An Introduction*, 2nd Ed., Chap. 10 & 11, John Wiley & Sons, 2009.
- R. Courant & D. Hilbert: *Methods of Mathematical Physics*, Vol. I, Chap. V, VI, & VII, Wiley-Interscience, 1953.
- D. S. Grebenkov & B.-T. Nguyen: “Geometrical structure of Laplacian eigenfunctions,” *SIAM Review*, vol. 55, no. 4, pp.601–667, 2013
- <https://www.math.ucdavis.edu/~saito/courses/LapEig/refs.html>
- Specific references are given throughout the lectures.

Outline

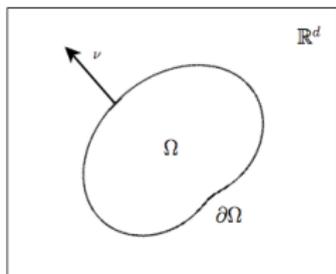
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Motivations: Why Irregular Domains?

- 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 $\Omega \implies$ need to avoid *the Gibbs phenomenon* due to $\partial\Omega$.
- Want to *represent* the object information efficiently for analysis, interpretation, discrimination, etc. \implies need *fast decaying* expansion coefficients relative to a *meaningful* basis.
- Want to extract and analyze *geometric information* about the domain $\Omega \implies$ M. Kac: “*Can one hear the shape of a drum?*” (1966); spectral geometry; shape clustering/classification.



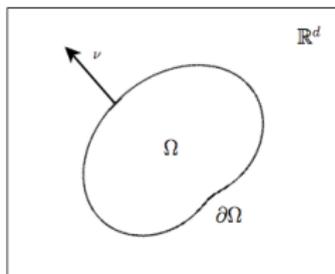
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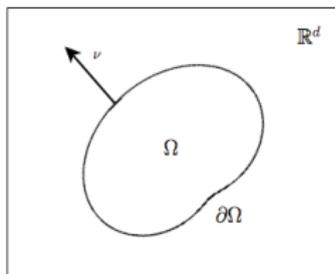
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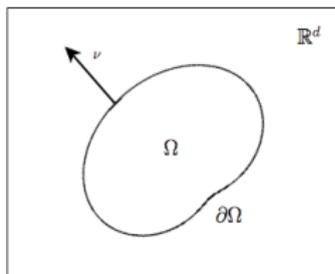
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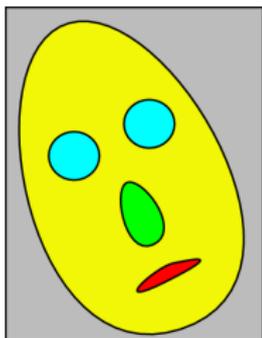


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Object-Oriented Image Analysis



(a) Original



(b) Background



(c) Object

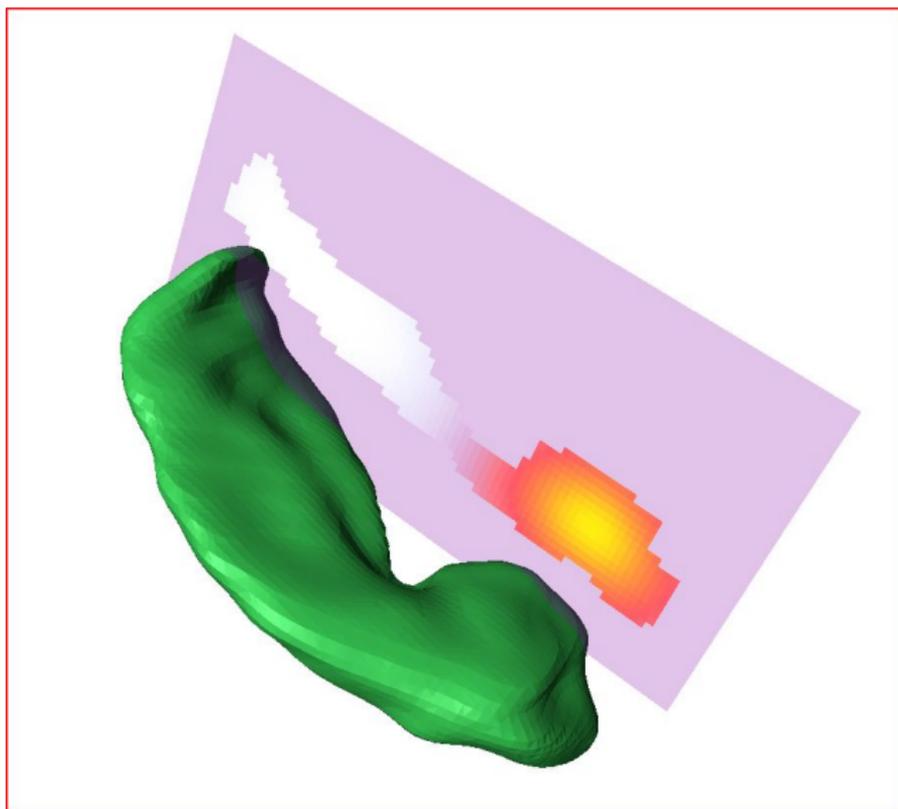


(d) Anomalies

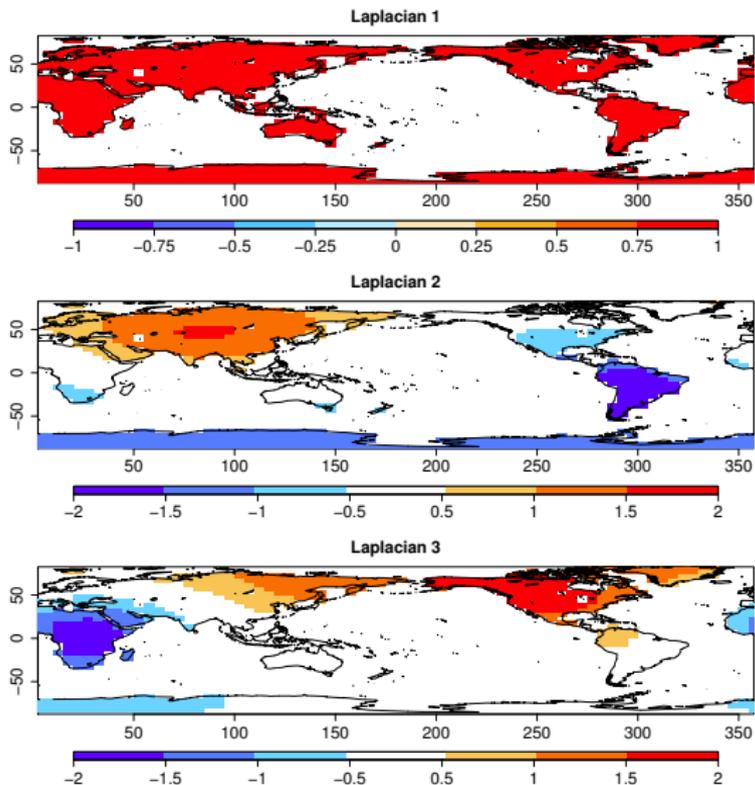
Data Analysis on a Complicated Domain



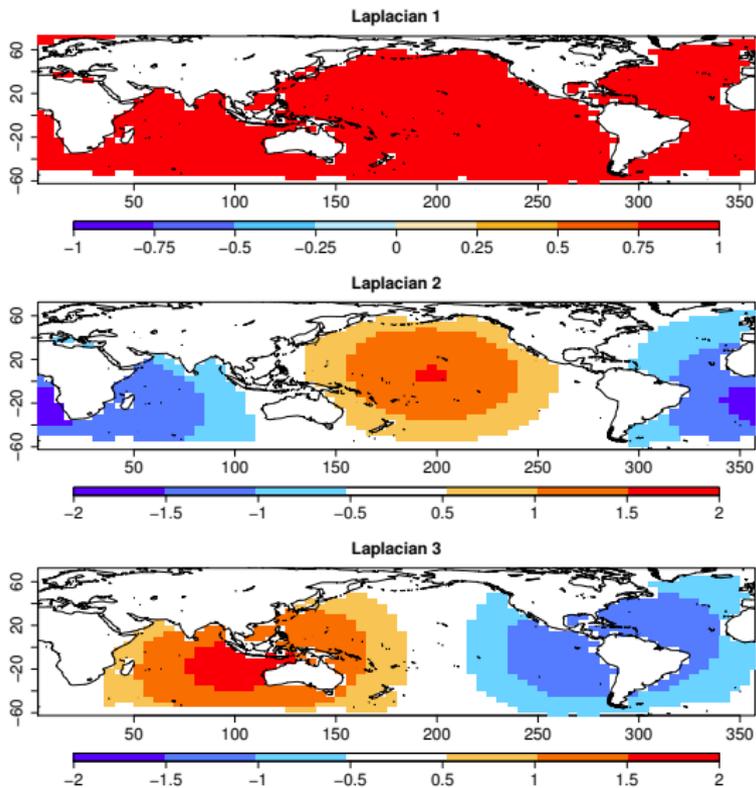
3D Hippocampus Shape Analysis (Courtesy: F. Beg)



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



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



Enter Laplacian Eigenfunctions!

- On irregular Euclidean domains, 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 $\mathcal{L} := -\Delta = -\left(\frac{\partial^2}{\partial x_1^2} + \dots + \frac{\partial^2}{\partial x_d^2}\right)$.
- The Laplacian eigenvalue problem is defined as:

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

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 $\partial\Omega$, $a \neq 0 \neq b$.

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Enter Laplacian Eigenfunctions . . .

- The nontrivial solution $u = \varphi$ of such a *boundary value problem* (BVP) is called the **Laplacian eigenfunction** corresponding to the eigenvalue λ .
- Via Green's 1st identity, the Dirichlet BC leads to:
 $0 < \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_k \rightarrow \infty$.
- On the other hand, the Neumann BC leads to:
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(a) P.-S. Laplace
(1749–1827)



(b) J.P.G.L. Dirichlet
(1805–1859)



(c) Carl Neumann
(1832–1925)



(d) Gustave Robin
(1855–1897)

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** \implies **Generalization of Fourier analysis!**

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Laplacian Eigenfunctions . . . Why?

- LEs have more **physical meaning** (i.e., vibration modes, heat conduction, . . .) than other popular basis functions such as *wavelets and wavelet packets*.
- LEs may particularly be useful for **inverse problems and imaging**: Suppose the domain shape Ω is **fixed** yet the material contents inside that domain, say $u(\mathbf{x})$, $\mathbf{x} \in \Omega$, change over time, i.e., $u(\mathbf{x}, t)$, $\mathbf{x} \in \Omega$, $t \in [0, T]$. Suppose one want to detect whether there is any change in the material contents in Ω over time, i.e., estimate $u_t(\mathbf{x}, t)$ via imaging.
- LEs may also be necessary for many **shape optimization** problems: e.g., among all possible 2D shapes having unit area, what is the shape that minimizes its *fifth* smallest Dirichlet-Laplacian eigenvalues?

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Shape Optimization (Courtesy of B. Osting)

Computational results for single eigenvalues

Oudet (2004)

No	Optimal union of discs	Computed shapes
3	 46.125	 46.125
4	 64.293	 64.293
5	 82.462	 78.47
6	 92.250	 88.96
7	 110.42	 107.47
8	 127.88	 119.9
9	 138.37	 133.52
10	 154.62	 143.45

Antunes + Freitas (2012)

i	Ω	multiplicity	λ_i^*	Oudet's result
5		2	78.20	78.47
6		3	88.52	88.96
7		3	106.14	107.47
8		3	118.90	119.9
9		3	132.68	133.52
10		4	142.72	143.45
11		4	159.39	-
12		4	172.85	-
13		4	186.97	-
14		4	198.96	-
15		5	209.63	-

- ▶ The level set method is used to represent the domains
- ▶ Relaxed formulation used to compute eigenvalues
- ▶ The k -th eigenvalue of the minimizer is multiple

- ▶ Eigenvalues computed via meshless method
- ▶ Domains parameterized using Fourier coefficients
- ▶ $k = 13$ minimizer is not symmetric

Laplacian Eigenfunctions . . . Some Facts

- Analysis of \mathcal{L} is difficult due to its unboundedness, etc.
- Much better to analyze its inverse, i.e., the Green's operator because it is **compact** and **self-adjoint**.
- Thus \mathcal{L}^{-1} has discrete spectra (i.e., a countable number of eigenvalues with finite multiplicity) except 0 spectrum.
- \mathcal{L} has a complete orthonormal basis of $L^2(\Omega)$, and this allows us to do **eigenfunction expansion** in $L^2(\Omega)$.

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- The key difficulty is to compute such eigenfunctions; directly solving the Helmholtz equation (or eigenvalue problem) on a general domain is tough.
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Laplacian Eigenfunctions in 1D — The Wave Equation

Around mid 18 C, d'Alembert, Euler, D. Bernoulli examined and created the theory behind vibrations of a 1D string.

- Consider a perfectly elastic and flexible string of length ℓ .
- $\rho(x)$: a mass density; $T(x)$: the tension of the string at $x \in [0, \ell]$.
- If $u(x, t)$ is the vertical displacement of the string at location $x \in [0, \ell]$ and time $t \geq 0$, then the string vibrates according to the **1D wave equation** (a.k.a. the **string equation**):
$$\rho(x) \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x} \left(T(x) \frac{\partial u}{\partial x} \right)$$

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- $\rho(x)$: a mass density; $T(x)$: the tension of the string at $x \in [0, \ell]$.
- If $u(x, t)$ is the vertical displacement of the string at location $x \in [0, \ell]$ and time $t \geq 0$, then the string vibrates according to the **1D wave equation** (a.k.a. the **string equation**):
$$\rho(x) \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x} \left(T(x) \frac{\partial u}{\partial x} \right)$$

Laplacian Eigenfunctions in 1D — The Wave Equation

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(a) Jean d'Alembert
(1717–1783)



(b) Leonhard Euler
(1707–1783)



(c) Daniel Bernoulli
(1700–1782)

Importance of the Boundary and Initial Conditions

- From now on, for simplicity, we assume the uniform density and constant tension, i.e., $\rho(x) \equiv \rho$, $T(x) \equiv T$.
- Under this assumption, the above wave equation simplifies to:

$$u_{tt} = c^2 u_{xx} \quad c \equiv \sqrt{T/\rho}.$$

- The 1D wave equation above has infinitely many solutions.
- Need to specify a boundary condition (BC) and an initial condition (IC) to obtain the desired solution.
- One possibility: both ends of the string are held fixed all the time \implies the **Dirichlet** BC: $u(0, t) = u(\ell, t) = 0$, $\forall t \geq 0$.
- As for the IC, let $u(x, 0) = f(x)$ (initial position); $u_t(x, 0) = g(x)$ (initial velocity), $\forall x \in [0, \ell]$. What we have then is:

$$\begin{cases} u_{tt} = c^2 u_{xx} & \text{for } x \in (0, \ell) \text{ and } t > 0; \\ u(0, t) = u(\ell, t) = 0 & \text{for } t \geq 0; \\ u(x, 0) = f(x), \quad u_t(x, 0) = g(x) & \text{for } x \in [0, \ell]. \end{cases} \quad (1)$$

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Behavior of the String $u(x, t)$

- Use the method of **separation of variables** to seek a nontrivial solution of the form: $u(x, t) = X(x)T(t)$.
- Plugging $X(x)T(t)$ into the (1), we get:

$$XT'' = c^2 X''T \implies \frac{X''}{X} = \frac{T''}{c^2 T} = k,$$

where k must be a *constant*.

- This leads to the following ODEs:

$$X'' - kX = 0 \quad \text{with } X(0) = X(\ell) = 0, \quad (2)$$

$$T'' - c^2 kT = 0 \quad (3)$$

- The characteristic equation of (2), i.e., $r^2 - k = 0$, must be analyzed carefully.

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Solving ODEs

Case I: $k > 0 \implies r = \pm\sqrt{k}$; hence

$$X(x) = Ae^{\sqrt{k}x} + Be^{-\sqrt{k}x} \quad \text{or} \quad A\cosh(\sqrt{k}x) + B\sinh(\sqrt{k}x).$$

Applying the BC $X(0) = X(\ell) = 0$ yields $A = B = 0$, thus the case of $k > 0$ is *not feasible*.

Case II: $k = 0 \implies X'' = 0 \implies X(x) = Ax + B$, which again leads to $X(x) \equiv 0$.

Case III: $k < 0$. Set $k = -\xi^2$ and $\xi > 0$. Then the characteristic equation becomes $r^2 + \xi^2 = 0$, i.e., $r = \pm i\xi$. Therefore we get

$$X(x) = A\cos(\xi x) + B\sin(\xi x)$$

By the BC $X(0) = X(\ell) = 0$, we get:

$$\begin{cases} X(0) = 0 & \implies A = 0 \\ X(\ell) = B\sin(\xi\ell) = 0 & \implies \xi = \frac{n\pi}{\ell}, \quad \forall n \in \mathbb{N} \end{cases}$$

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Forming the Solution

- Hence we have $X(x) = B \sin\left(\frac{n\pi}{\ell} x\right)$, and for convenience, by setting $B = \sqrt{2/\ell}$, let us define

$$X_n(x) = \varphi_n(x) := \sqrt{\frac{2}{\ell}} \sin\left(\frac{n\pi}{\ell} x\right),$$

so that $\|\varphi_n\|_{L^2[0,\ell]} = 1$. Note that $\{\varphi_n\}_{n \in \mathbb{N}}$ form an **orthonormal basis** for $L^2[0,\ell]$.

- Similarly, by $T'' = -\xi^2 c^2 T$ we obtain the family of solutions

$$T_n(t) = a_n \cos\left(\frac{n\pi c}{\ell} t\right) + b_n \sin\left(\frac{n\pi c}{\ell} t\right).$$

- Now, for each $n \in \mathbb{N}$, the function

$$u_n(x, t) = T_n(t) \cdot \varphi_n(x) = \left\{ a_n \cos\left(\frac{n\pi c}{\ell} t\right) + b_n \sin\left(\frac{n\pi c}{\ell} t\right) \right\} \sqrt{\frac{2}{\ell}} \sin\left(\frac{n\pi}{\ell} x\right)$$

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- Hence, by the *Superposition Principle*,

$$u(x, t) = \sum_{n=1}^{\infty} u_n(x, t) = \sum_{n=1}^{\infty} \left\{ a_n \cos\left(\frac{n\pi c}{\ell} t\right) + b_n \sin\left(\frac{n\pi c}{\ell} t\right) \right\} \varphi_n(x) \quad (4)$$

is a general solution with yet undetermined coefficients a_n and b_n .

- Next, we specify the coefficients a_n and b_n by matching (4) with the ICs in (1). Thus we get

$$u(x, 0) = f(x) = \sum_{n=1}^{\infty} a_n \sqrt{\frac{2}{\ell}} \sin\left(\frac{n\pi}{\ell} x\right) = \sum_{n=1}^{\infty} a_n \varphi_n(x)$$

Then

$$a_n = \langle f, \varphi_n \rangle = \sqrt{\frac{2}{\ell}} \int_0^{\ell} f(x) \sin\left(\frac{n\pi}{\ell} x\right) dx,$$

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- Note that $\frac{n\pi c}{\ell} b_n = \langle g, \varphi_n \rangle \implies b_n = \frac{\ell}{n\pi c} \langle g, \varphi_n \rangle$.

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Figure: Jean Baptiste Joseph Fourier (1768–1830)

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Remarks

- Need to check if our solution makes sense physically. Notice that

$$c^2 = \frac{T}{\rho} \implies \text{the sound frequency} = \frac{n\pi}{\ell} \sqrt{\frac{T}{\rho}}.$$

- Hence, ℓ is short, T is high, and ρ is small (thin), then such a string generates a high frequency tone.
- On the other hand, if ℓ is long, T is low, and ρ is large (thick), then it generates a low frequency tone.
- Note that the Neumann BC imposes

$$u_x(0, t) = u_x(\ell, t) = 0 \quad \forall t > 0.$$

This leads to the Fourier cosine series expansions of f and g . Note that the Neumann problem allows the solution $u_0(x, t) = a_0 = \text{const.}$

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This leads to the **Fourier cosine series expansions** of f and g . Note that the Neumann problem allows the solution $u_0(x, t) = a_0 = \text{const.}$

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- Through the separation of variables for finding a solution to the 1D string equation with BC & IC (1), we arrive at the system

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- Notice that (5) is a 1D version of the **Dirichlet-Laplacian** eigenvalue problem with $\Omega = (0, \ell)$.
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- For instance, the size of the first eigenvalue, $\lambda_1 = (\pi/\ell)^2$ tells us the **volume** of Ω (i.e., the length ℓ of Ω in 1D).
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Outline

- 1 Motivations
- 2 History of Laplacian Eigenvalue Problems – Spectral Geometry
 - 1D Wave Equation
 - Spectral Geometry 101
- 3 Harmonic Analysis of/on Irregular Domains via Eigenfunctions of Integral Operators Commuting with Laplacians
- 4 Summary & References

Spectral Geometry 101

- The Laplacian eigenfunctions defined on the domain Ω provides the orthonormal basis of $L^2(\Omega)$.
- The Laplacian eigenvalues encode geometric information of the domain $\Omega \implies$ “Can we hear the shape of a drum?” (Mark Kac, 1966).
- Temporarily, consider the Laplacian eigenvalue problem on a planar domain $\Omega \in \mathbb{R}^2$ with the *Dirichlet* boundary condition:

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(a) Hermann Weyl
(1885–1955)



(b) S. Minakshisundaram



(c) Åke Pleijel
(1913–1989)



(d) Mark Kac
(1914–1984)

Universal (or Payne-Pólya-Weinberger) Inequalities ($m \in \mathbb{N}$)

- $\lambda_{m+1} - \lambda_m \leq 2 \cdot \frac{1}{m} \sum_{j=1}^m \lambda_j$; $\lambda_{m+1} \leq 3 \cdot \frac{1}{m} \sum_{j=1}^m \lambda_j$; $\frac{\lambda_{m+1}}{\lambda_m} \leq 3$.
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(a) L. E. Payne (1923–2011)



(b) G. Pólya (1887–1985)



(c) H. Weinberger (1928–)

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- $\frac{\lambda_2}{\lambda_1} \leq \frac{j_{1,1}^2}{j_{0,1}^2} \approx 2.5387$ (Ashbaugh-Benguria)
- $j_{k,1}$ is the first zero of the Bessel function of order k , i.e., $J_k(j_{k,1}) = 0$.
 $j_{0,1} \approx 2.4048$, $j_{1,1} \approx 3.8317$, and $|\Omega|$ is the area of Ω . In both cases, the equality is attained iff Ω is a disk in \mathbb{R}^2 .

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(a) Lord Rayleigh
(1842–1919)



(b) Georg Faber
(1877–1966)



(c) Edgar Krahn
(1894–1961)



(d) Mark
Ashbaugh (1953–)



(e) Rafael
Benguria (1951–)

Remarks

Excellent references on these inequalities are:

- R. D. Benguria, H. Linde, & B. Loewe: “Isoperimetric inequalities for eigenvalues of the Laplacian and the Schrödinger operator,” *Bull. Math. Sci.*, vol. 2, pp. 1–56, 2012.
- A. Henrot: *Extremum Problems for Eigenvalues of Elliptic Operators*, Birkhäuser Verlag, Basel, 2006.

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- Laplacian eigenvalues are *translation and rotation invariant*.
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An Counterexample to the Domain Monotonicity

Consider a 2D rectangle of sides a and b with $a > b$. Then, let $\Omega' := \{(x, y) \mid 0 < x < a, 0 < y < b\}$, and $\Omega \subset \Omega'$ be the inscribed thin rectangle of sides $\sqrt{\alpha^2 + \beta^2} \times \sqrt{(a - \alpha)^2 + (b - \beta)^2}$:

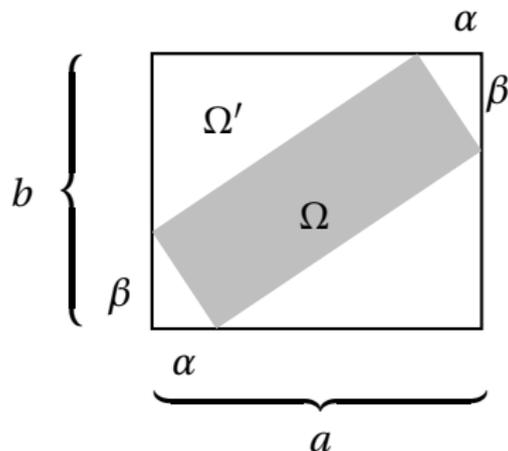


Figure: The Neumann BC generates an counterexample (From A. Henrot, 2006)

An Counterexample to the Domain Monotonicity ...

- Can easily compute the Neumann eigenvalues and eigenfunctions for a rectangle Ω' :

$$\lambda_n^N = \lambda_{\ell,m}^N = \pi^2 \left[\left(\frac{\ell}{a} \right)^2 + \left(\frac{m}{b} \right)^2 \right],$$

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where $c_0 := 2/\sqrt{ab}$.

- Clearly, the smallest eigenvalue is: $\lambda_0^N = \lambda_{0,0}^N = 0$, $\varphi_0^N(x, y) \equiv c_0$.
- How about the next smallest one? Since $a > b$,

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- 2 History of Laplacian Eigenvalue Problems – Spectral Geometry
- 3 Harmonic Analysis of/on Irregular Domains via Eigenfunctions of Integral Operators Commuting with Laplacians**
- 4 Summary & References

Numerical Methods for Laplacian Eigenvalue Problems

- **Finite Difference Method (FDM)**
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 - **Integral Operators Commuting with Laplacian**
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 - Image Approximation I: Comparison with Wavelets
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Recap on Difficulties Dealing with Laplacian

- Analysis of the Laplacian $\mathcal{L} = -\Delta$ is difficult due to its unboundedness, etc.
- Computing the eigenfunctions of \mathcal{L} by directly solving the Helmholtz equation (or eigenvalue problem) on a general domain is tough.
- Much better to analyze its inverse, i.e., the Green's operator because it is **compact** and **self-adjoint**.
- Unfortunately, computing the Green's function for a general Ω satisfying the usual boundary condition (i.e., Dirichlet, Neumann) is also very difficult.

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Integral Operators Commuting with Laplacian

- The key idea to avoid difficulties associated with the Laplacian \mathcal{L} is to find an integral operator \mathcal{K} *commuting* with \mathcal{L} without imposing the strict boundary condition a priori.
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Theorem (G. Frobenius 1896?; B. Friedman 1956)

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



(a) G. Frobenius (1849–1917)



(b) B. Friedman (1915–1966)

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

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

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.

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

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

Theorem (NS 2005, 2008)

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

$$\int_{\partial\Omega} K(\mathbf{x}, \mathbf{y}) \frac{\partial\varphi}{\partial\nu_{\mathbf{y}}}(\mathbf{y}) ds(\mathbf{y}) = -\frac{1}{2}\varphi(\mathbf{x}) + \text{pv} \int_{\partial\Omega} \frac{\partial K(\mathbf{x}, \mathbf{y})}{\partial\nu_{\mathbf{y}}} \varphi(\mathbf{y}) ds(\mathbf{y}), \quad \forall \mathbf{x} \in \partial\Omega,$$

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 $\varphi(\mathbf{x})$ of the integral operator \mathcal{K} in the previous theorem can be **extended** outside the domain Ω and satisfies the following equation:

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

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

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

Integral Operators Commuting with Laplacian ...

Corollary (NS 2005, 2008)

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

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

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

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1D Example

- Consider the unit interval $\Omega = (0, 1)$.
- Then, our integral operator \mathcal{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 $K(x, y)$ is of *Toeplitz* form \implies Eigenvectors must have even and odd symmetry (Cantoni-Butler '76).
- In this case, we have the following explicit solution.

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1D Example ...

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

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

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

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

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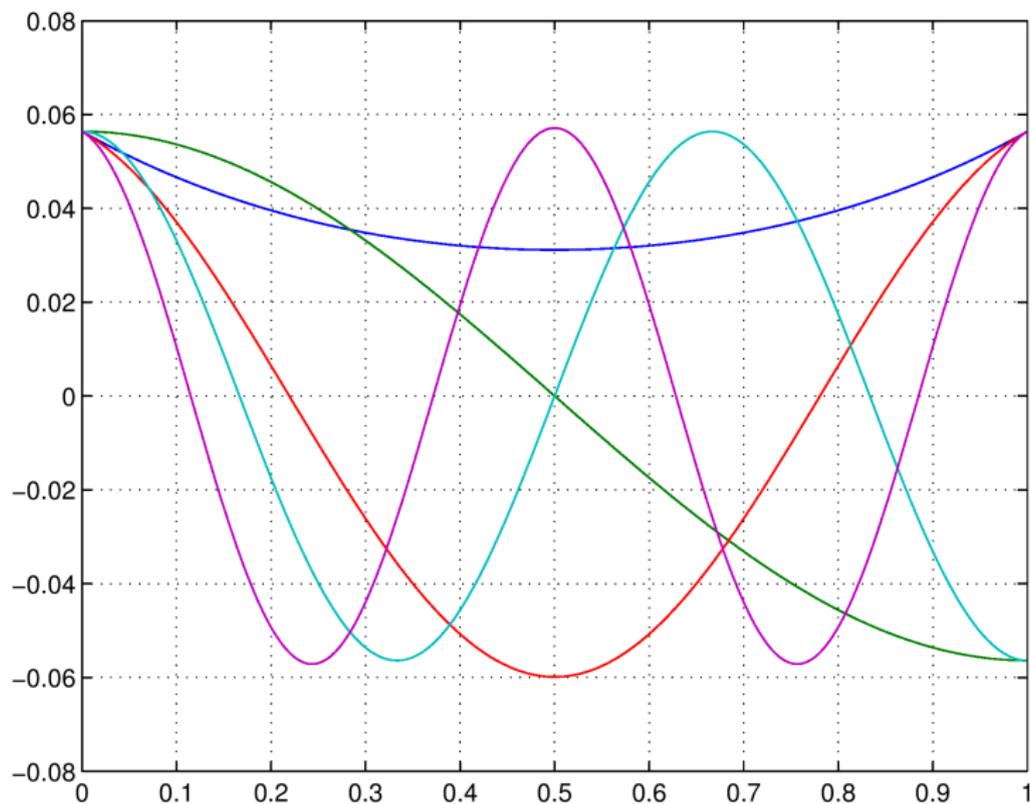
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First 5 Basis Functions



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 \Leftrightarrow DST-I/DCT-I;
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2D Example

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

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

$$\frac{\partial\varphi}{\partial\nu}\Big|_{\partial\Omega} = \frac{\partial\varphi}{\partial r}\Big|_{\partial\Omega} = -\frac{\partial\mathcal{H}\varphi}{\partial\theta}\Big|_{\partial\Omega},$$

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

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

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

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

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

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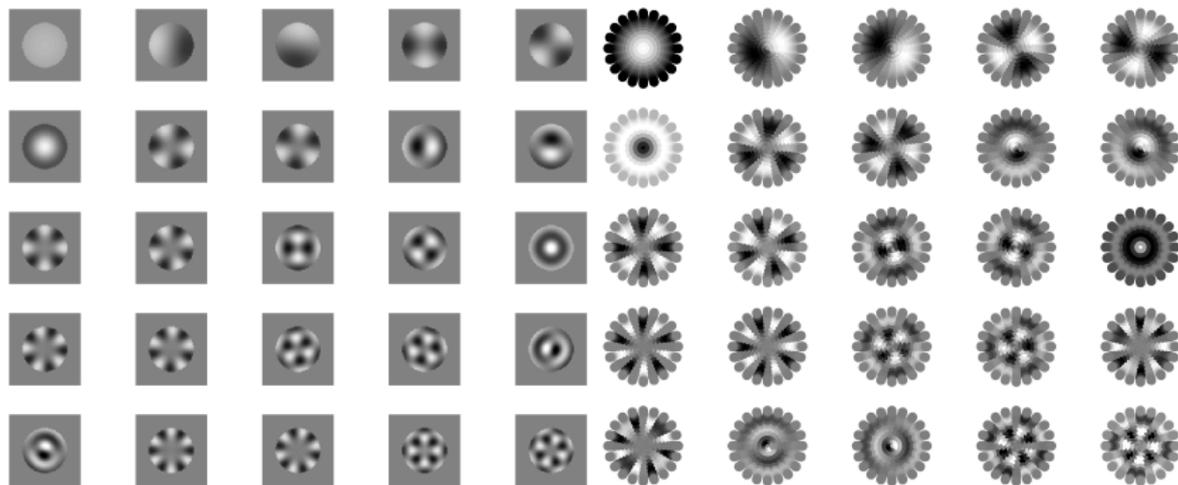
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First 25 Basis Functions

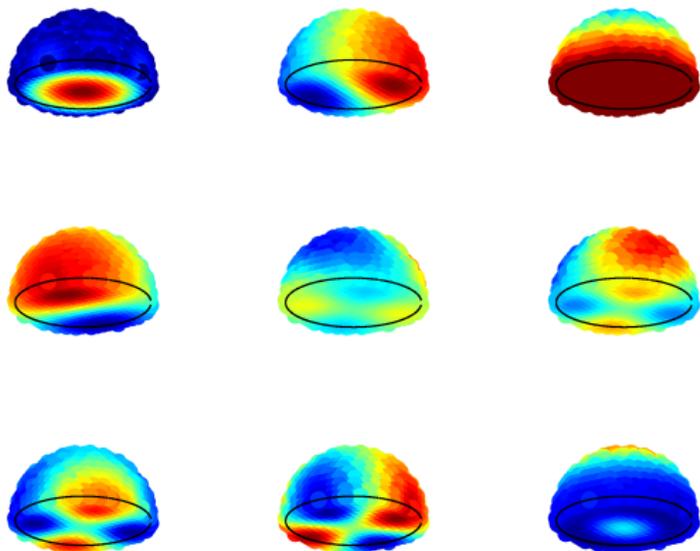


(a) Our Basis

(b) Dirichlet-Laplace

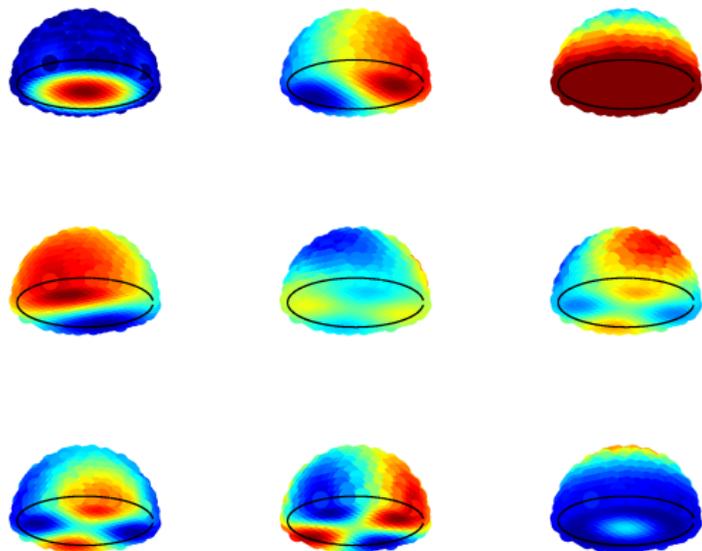
3D Example

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



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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 $\{\mathbf{x}_i\}_{i=1}^N$.
- Under these assumptions, we can approximate the integral eigenvalue problem $\mathcal{K}\varphi = \mu\varphi$ with a simple quadrature rule with node-weight pairs (\mathbf{x}_j, w_j) as follows.

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

- Let $K_{i,j} := w_j K(\mathbf{x}_i, \mathbf{x}_j)$, $\varphi_i := \varphi(\mathbf{x}_i)$, and $\boldsymbol{\varphi} := (\varphi_1, \dots, \varphi_N)^\top \in \mathbb{R}^N$. 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**.

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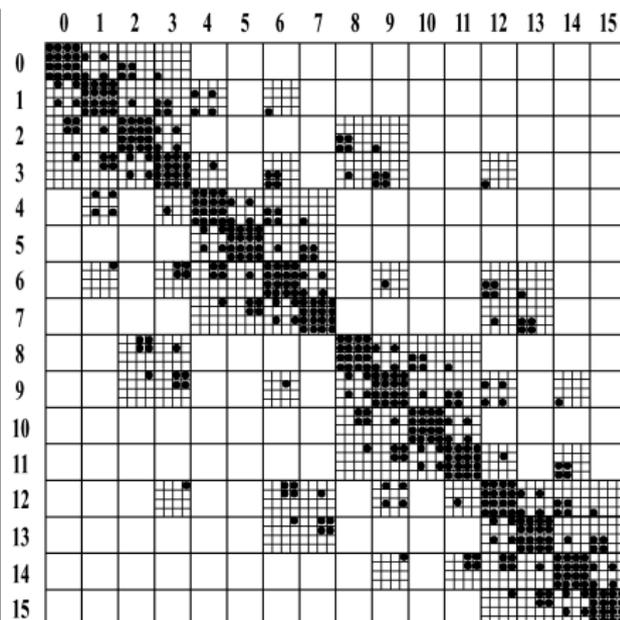
A Possible Fast Algorithm for Computing φ_j 's

- Observation: our kernel function $K(\mathbf{x}, \mathbf{y})$ 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

0	1	4	5	16	17	20	21
0			1		4		5
2	3	0	6	7	18	19	1
8	9		3	12	13	24	25
2					6		7
10	11	14	15	26	27	30	31
32	33	36	37	48	49	52	53
8		9		12		13	
34	35	2	38	39	50	51	3
40	41		4	44	45	56	57
10		11		14		15	
42	43	46	47	58	59	62	63

(a) Hierarchical indexing scheme

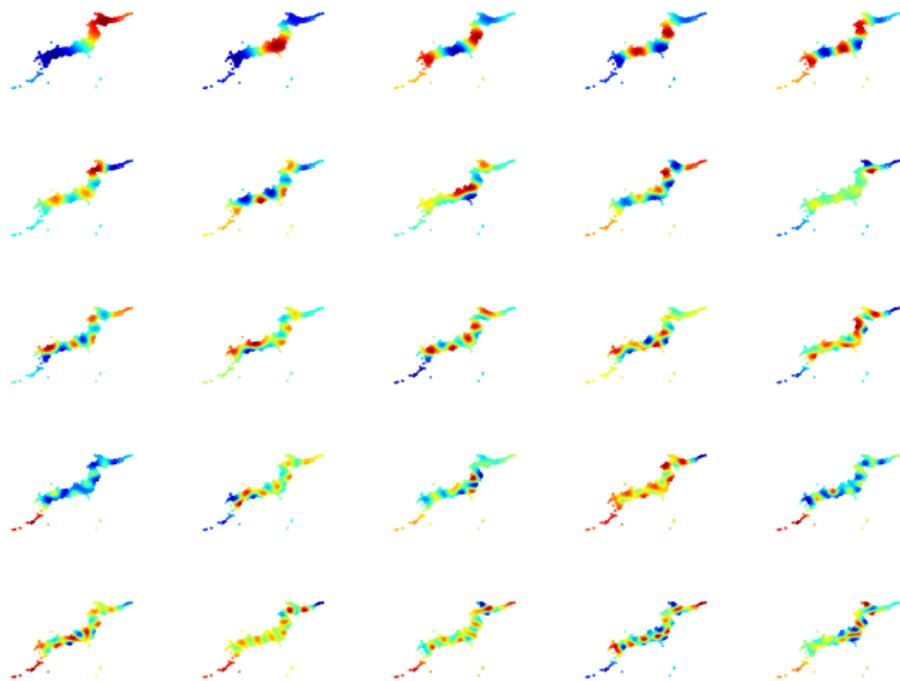


(b) Tree-Structured Matrix

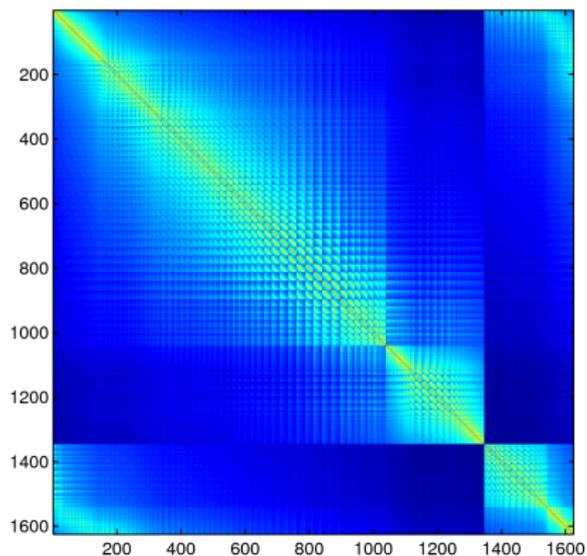
A Real Challenge: Kernel matrix is of 387924×387924 .



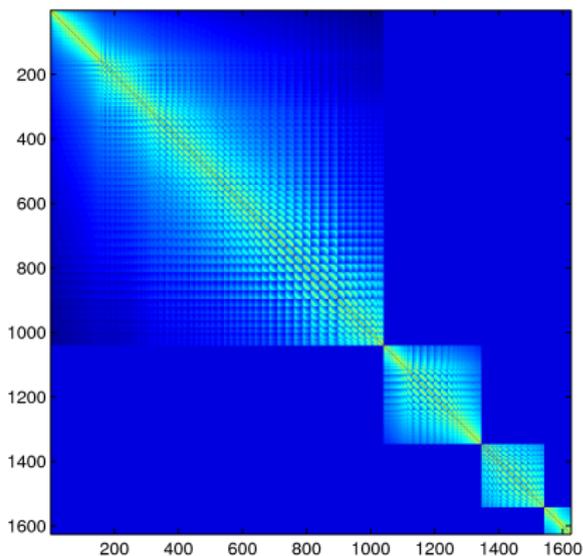
First 25 Basis Functions via the FMM-based algorithm



Splitting into Subproblems for Faster Computation

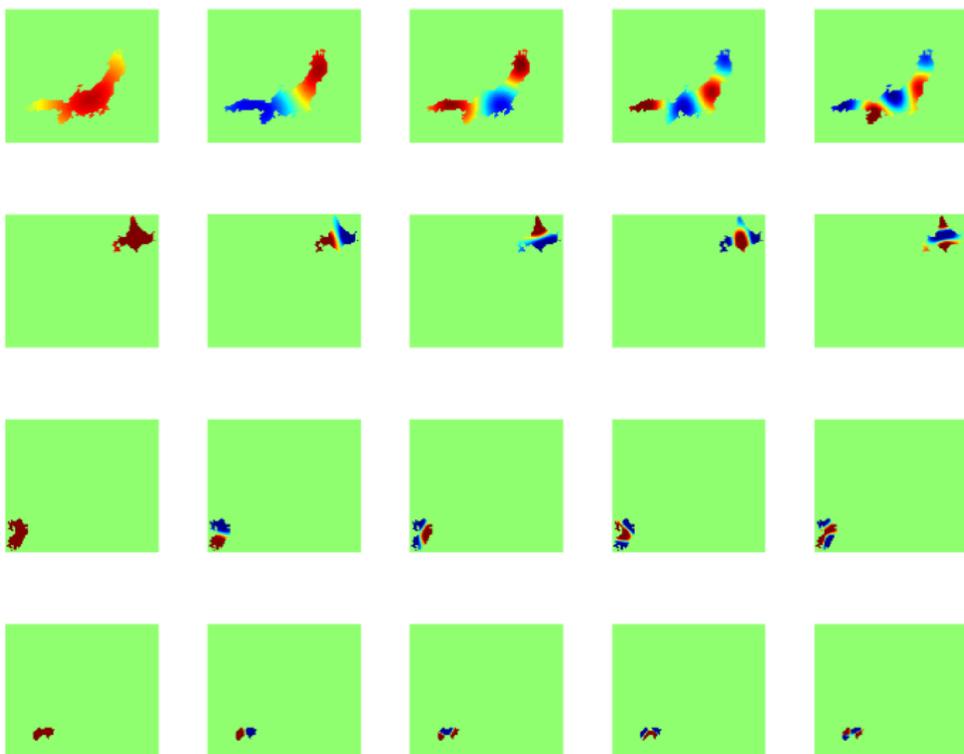


(a) Whole islands



(b) Separated islands

Eigenfunctions for Separated Islands



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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.
- ...

Remark on the DC vector

- The Laplacian eigenfunction with the least oscillation computed by diagonalizing the commuting integral operator is *not* the constant (i.e., DC) vector $\chi_\Omega := \mathbf{1}_N / \sqrt{N} \in \mathbb{R}^N$.
- If some application needs to have the DC vector of a given domain Ω and the basis vectors orthogonal to the DC vector, there is a way to include the DC vector into the picture.
- Consider the *orthogonal complement* to the 1D subspace $\text{span}\{\chi_\Omega\}$ in the column space of the kernel matrix K :

$$\tilde{K} = (I - \chi_\Omega \chi_\Omega^\top) K.$$

- Then, χ_Ω together with the eigenvectors of \tilde{K} corresponding to the largest $N - 1$ eigenvalues form the desired orthonormal basis.

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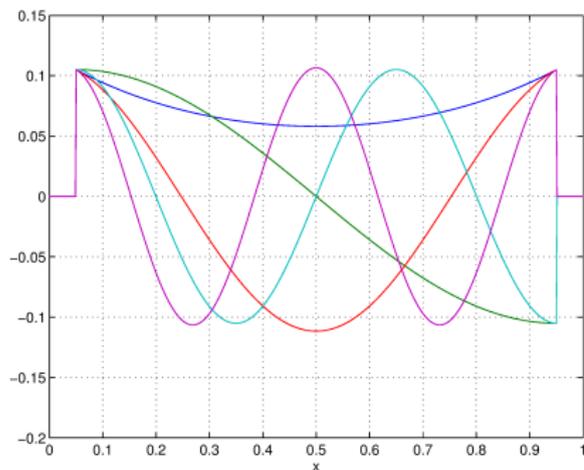
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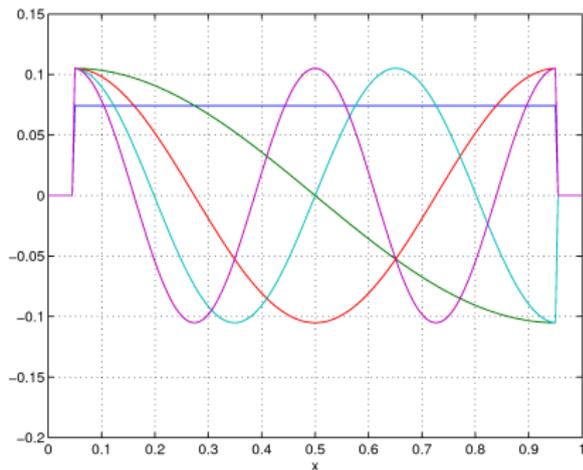
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Remark on the DC vector ...



(a) Laplacian Eigenfunctions via Commuting Integral Operator



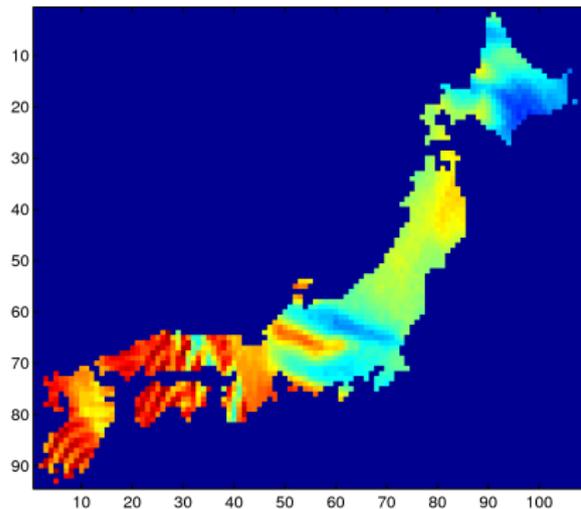
(b) Laplacian Eigenfunctions incorporating the DC vector

⇒ leads to the *generalized discrete cosine basis!*

Outline

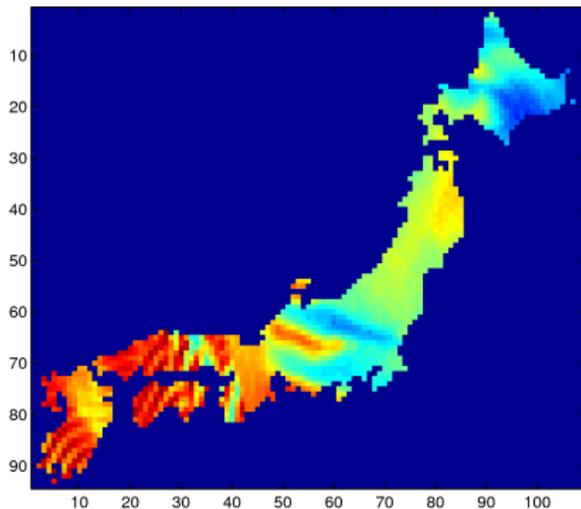
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Image Approximation; Comparison with Wavelets

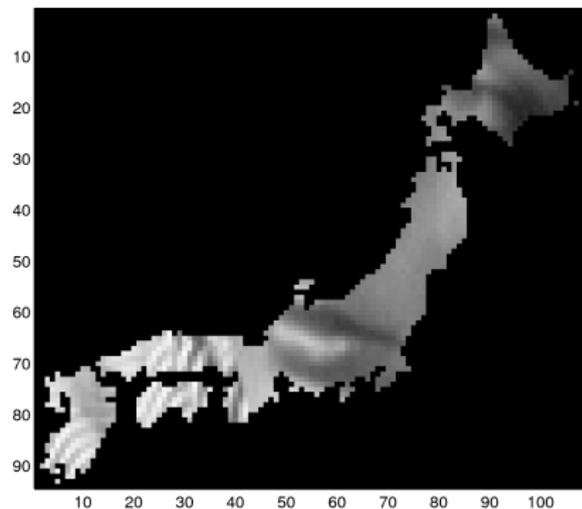


(a) What data?

Image Approximation; Comparison with Wavelets

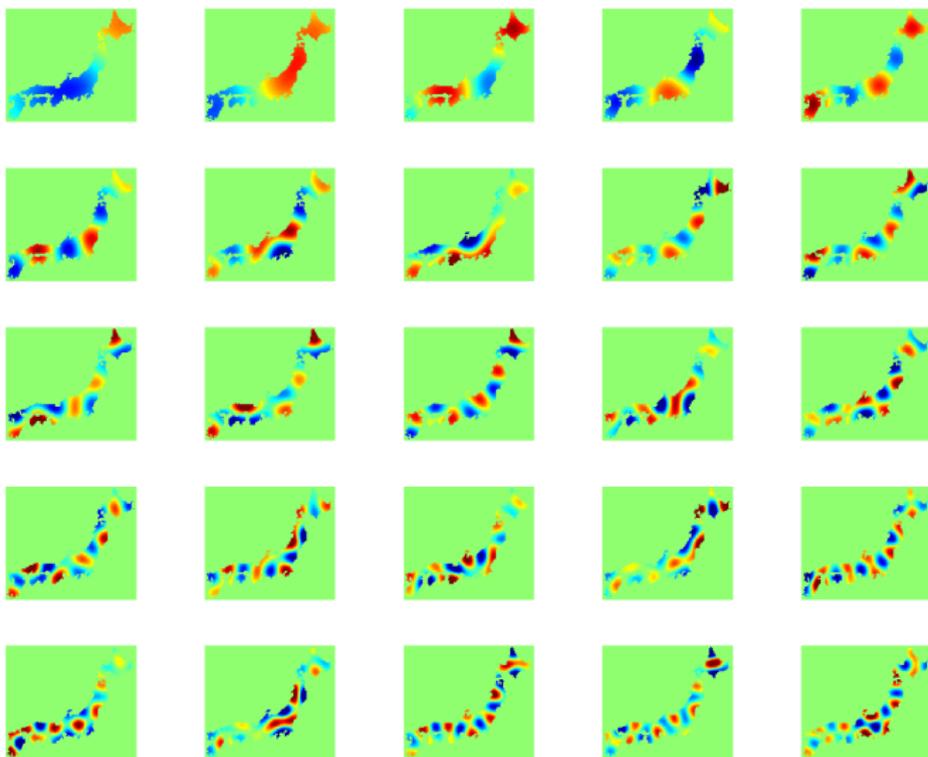


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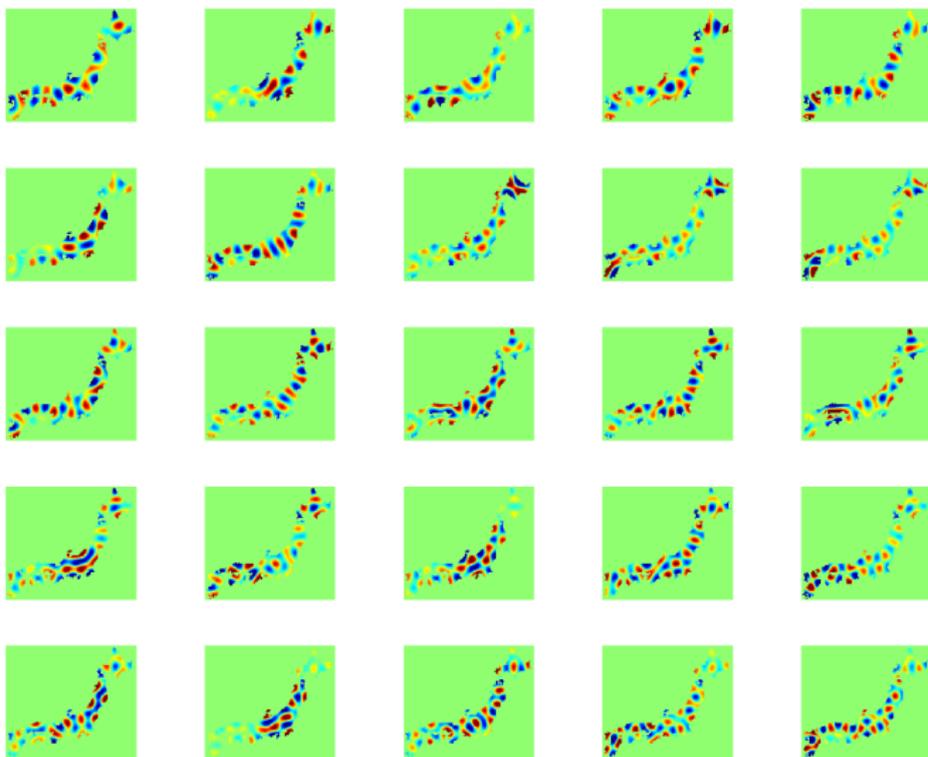


(b) $\chi_J \cdot \text{Barbara}$

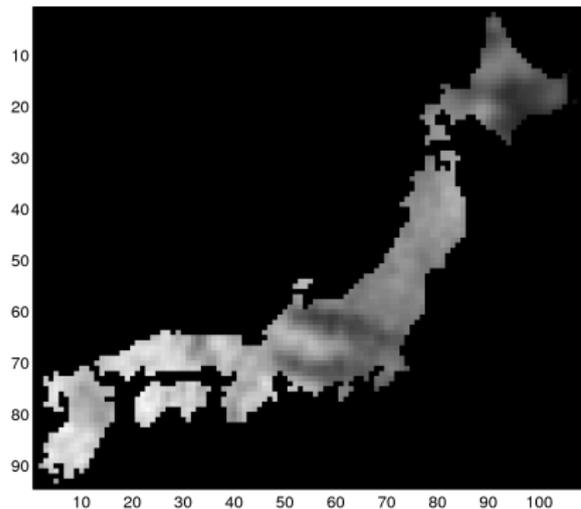
First 25 Basis Functions



Next 25 Basis Functions

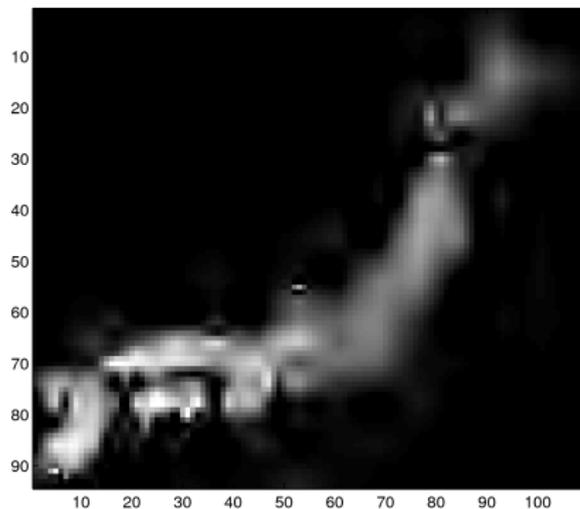


Reconstruction with Top 100 Coefficients



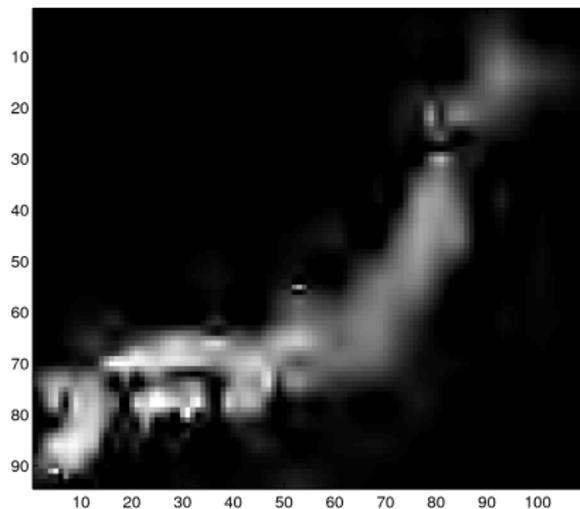
(a) Reconstruction

Reconstruction with Top 100 2D Wavelets (Symmlet 8)

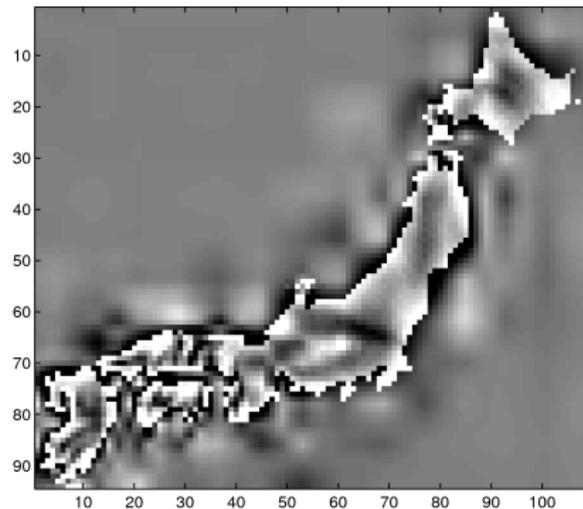


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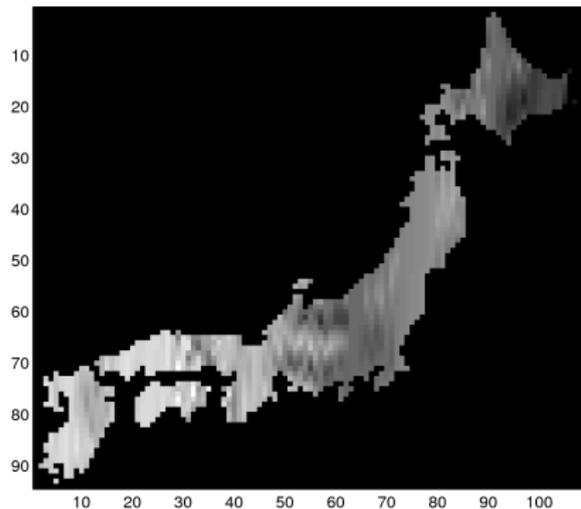


(a) Reconstruction



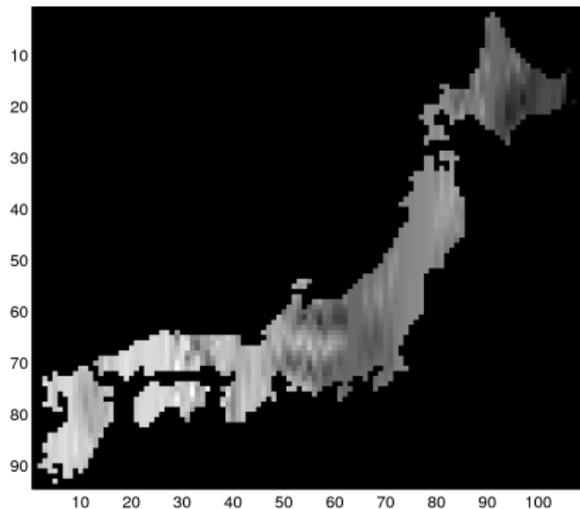
(b) Error

Reconstruction with Top 100 1D Wavelets (Symmlet 8)

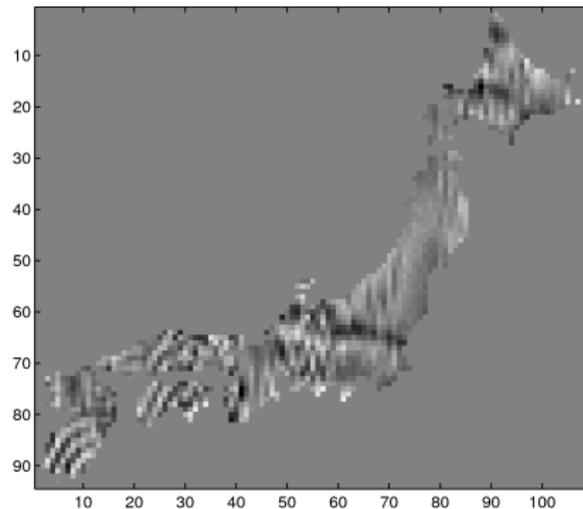


(a) Reconstruction

Reconstruction with Top 100 1D Wavelets (Symmlet 8)

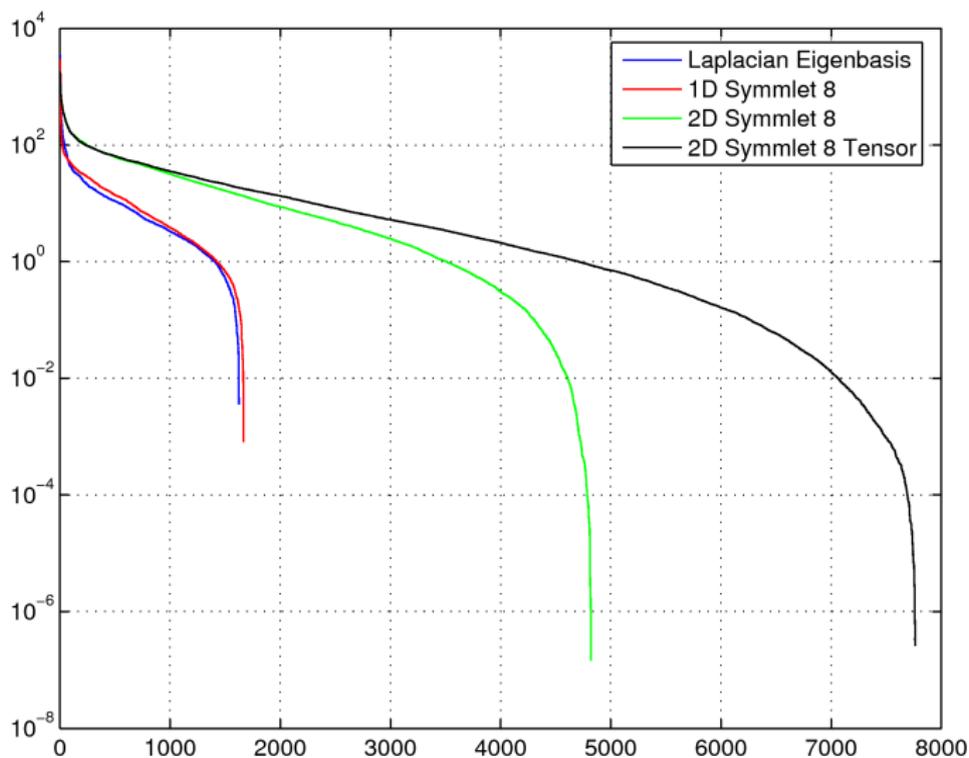


(a) Reconstruction



(b) Error

Comparison of Coefficient Decay



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 - **Image Approximation II: Robustness against Perturbed Boundaries**
 - Hippocampal Shape Analysis
 - Statistical Image Analysis; Comparison with PCA
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Experiments on Domains with Perturbed Boundaries

We will use the following domains for our experiments:

Ω_1 : The Japanese Islands

Ω_2 : A smoothed and connected version of Ω_1 ;

Ω_3 : The same as Ω_2 but with a “jaggy” boundary curve

Ω_4 : The two-component version of Ω_2 .

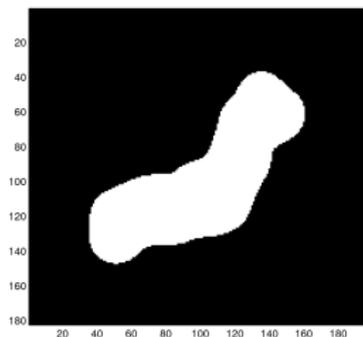
As for the data on these domains, we adopted three functions with different smoothness:

- 1 A discontinuous function (i.e., a simple step function whose discontinuity is a straight line along the “spine” or the main axis of the domain);
- 2 A pyramid-shaped function, which is continuous and its first order partial derivatives are of bounded variation;
- 3 The standard Gaussian function.

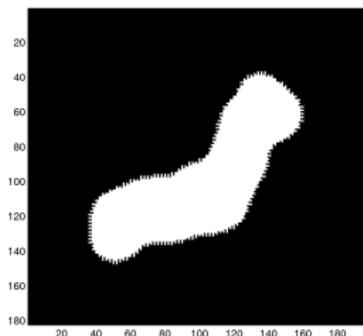
The Domains with Perturbed Boundaries



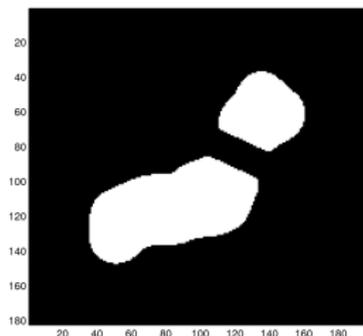
(a) χ_{Ω_1}



(b) χ_{Ω_2}

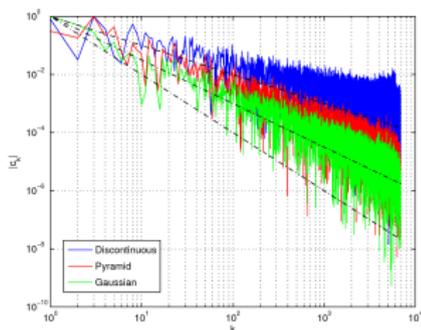
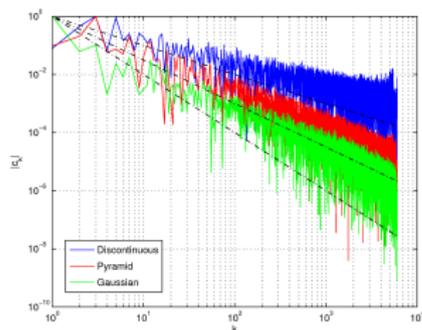
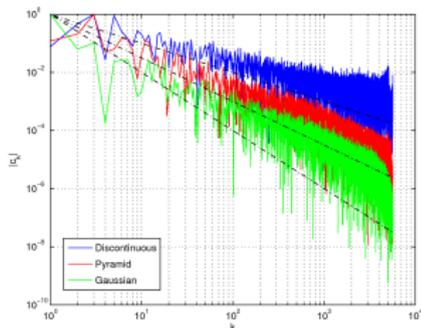
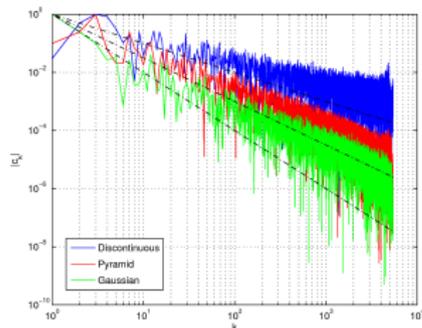


(c) χ_{Ω_3}



(d) χ_{Ω_4}

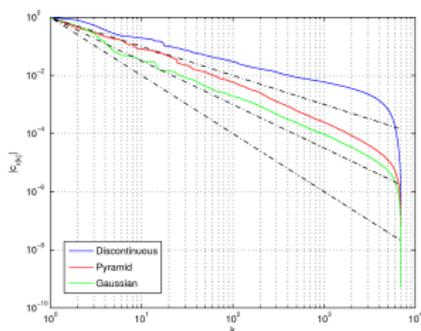
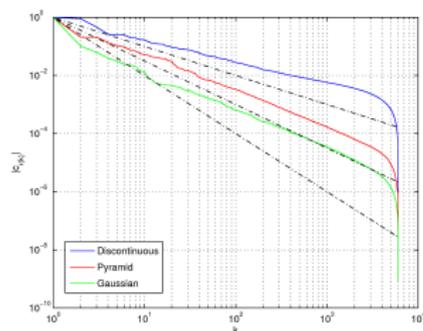
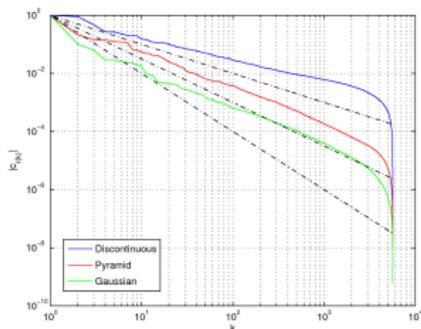
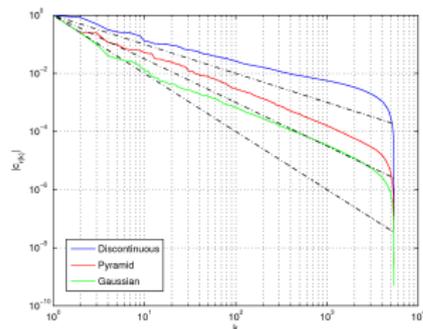
Decay Rates of the Expansion Coefficients (Unsorted)

(a) Decay rates on Ω_1 (b) Decay rates on Ω_2 (c) Decay rates on Ω_3 (d) Decay rates on Ω_4

Observations on the Decay Rates

- The decay rates reflect the intrinsic smoothness of the functions living in the domain, but are not affected by the existence of the boundary of the domains.
- The decay rates are rather insensitive to the smoothness of the boundary curves. In particular, the plots for Ω_2 , Ω_3 , and Ω_4 are virtually the same whereas those for Ω_1 —the most complicated domain among these four—seem slightly worse than the others. Yet all behave better than $O(k^{-1})$.
- The decay rates are rather insensitive to the number of the separated subdomains. Again, it will be also of interest to investigate the behavior the conventional Laplacian eigenfunctions in this respect.
- Although the coefficient plots oscillate around the linear lines (in the log-log scale), the decay rates $O(k^{-\alpha})$, regardless of the domain shapes, behave as follows. For the discontinuous functions, $\alpha < 1$. For the pyramid-shape function, $1 < \alpha < 1.5$. For the Gaussian function, $\alpha \geq 1.5$.

Decay Rates of the Expansion Coefficients (Sorted)

(a) Decay rates on Ω_1 (b) Decay rates on Ω_2 (c) Decay rates on Ω_3 (d) Decay rates on Ω_4

Conjecture on the Coefficient Decay Rate

Conjecture (NS 2007)

Let Ω be a C^2 -domain of general shape and let $f \in C(\overline{\Omega})$ with $\frac{\partial f}{\partial x_j} \in BV(\overline{\Omega})$ for $j = 1, \dots, d$. Let $\{c_k = \langle f, \varphi_k \rangle\}_{k \in \mathbb{N}}$ be the expansion coefficients of f with respect to our Laplacian eigenbasis on this domain. Then, $|c_k|$ decays with rate $O(k^{-\alpha})$ with $1 < \alpha < 2$ as $k \rightarrow \infty$. Thus, the approximation error using the first m terms measured in the L^2 -norm, i.e., $\|f - \sum_{k=1}^m c_k \varphi_k\|_{L^2(\Omega)}$ should have a decay rate of $O(m^{-\alpha+0.5})$ as $m \rightarrow \infty$.

The C^2 -smoothness of the boundary could be weakened ...

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The C^2 -smoothness of the boundary could be weakened ...

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- 1 Motivations
- 2 History of Laplacian Eigenvalue Problems – Spectral Geometry
- 3 **Harmonic Analysis of/on Irregular Domains via Eigenfunctions of Integral Operators Commuting with Laplacians**
 - Integral Operators Commuting with Laplacian
 - Simple Examples
 - Discretization of the Problem
 - Fast Algorithms for Computing Eigenfunctions
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Hippocampal Shape Analysis

- Presenting the work of *Faisal Beg* and his group at Simon Fraser Univ. using our technique
- Want to distinguish people with mild dementia of the Alzheimer type (DAT) from cognitively normal (CN) people
- Hippocampus plays important roles in long-term memory and spatial navigation

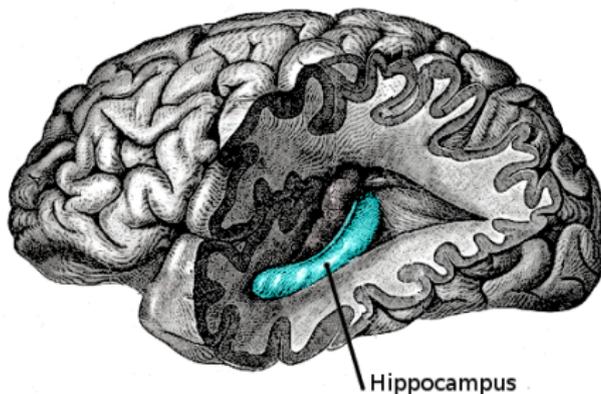


Figure: From Wikipedia

Hippocampal Shape Analysis . . .

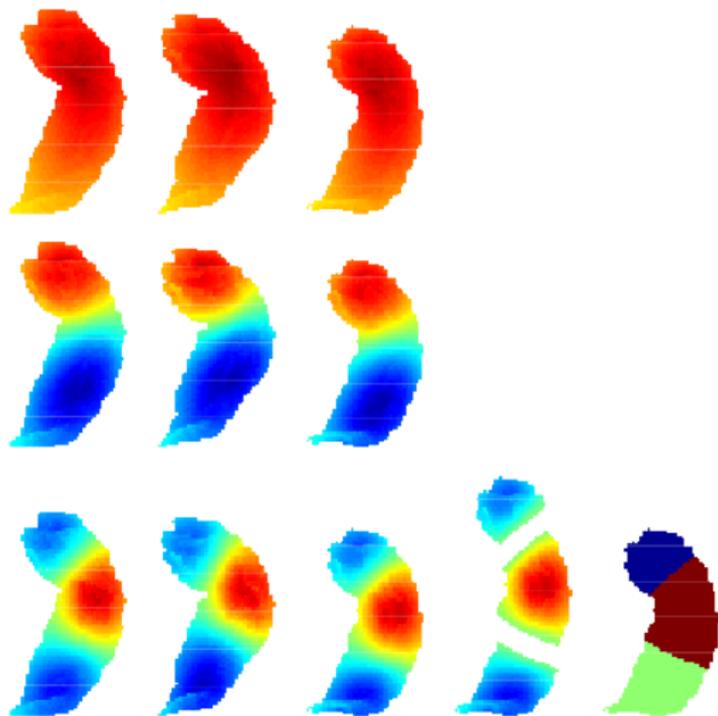
- Dataset: Left hippocampus segmented from 3D MRI images
- Compute the smallest 999 Laplacian eigenvalues (i.e., the largest 999 eigenvalues of the integral operator \mathcal{K}) for each left hippocampus
- Construct a feature vector for each left hippocampus:

$$\mathbf{F} := \left(\frac{\lambda_1}{\lambda_2}, \dots, \frac{\lambda_1}{\lambda_{n+1}} \right)^\top = \left(\frac{\mu_2}{\mu_1}, \dots, \frac{\mu_{n+1}}{\mu_1} \right)^\top \in \mathbb{R}^n.$$

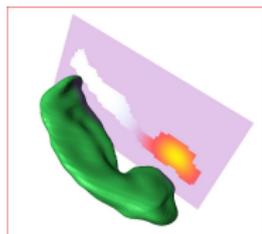
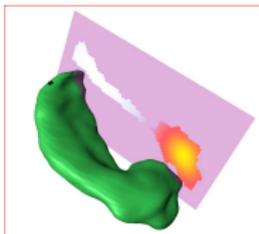
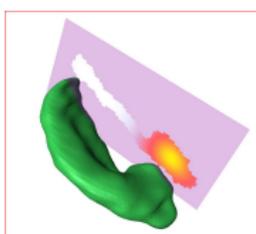
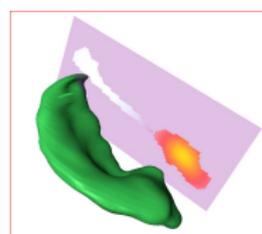
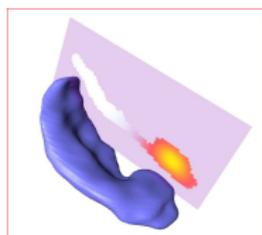
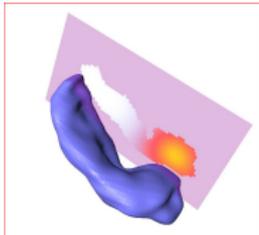
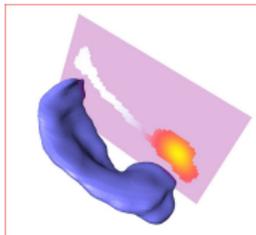
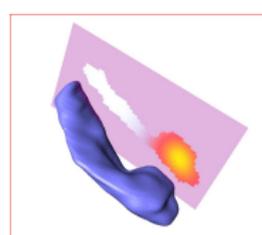
This feature vector was used by Khabou, Hermi, and Rhouma (2007) for 2D shape classification (e.g., shapes of tree leaves).

- Reduce the feature space dimension via PCA to from $n = 998$ to n'
- Classified by the linear SVM (support vector machine)

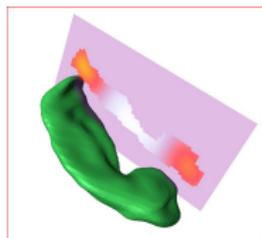
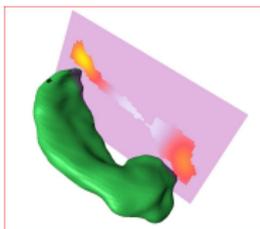
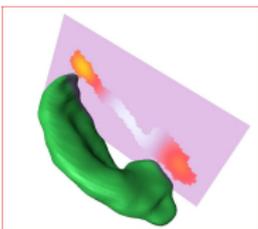
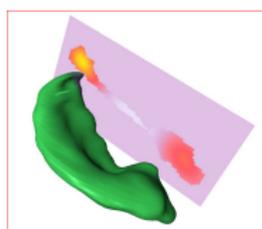
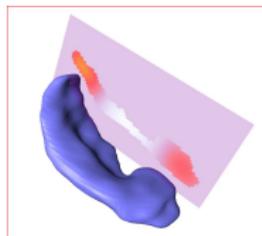
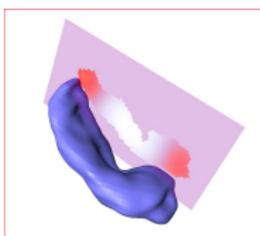
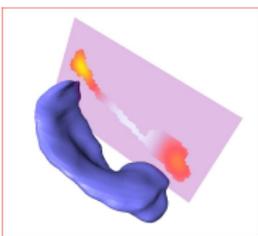
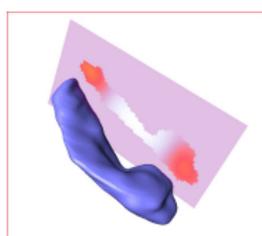
First Three Eigenfunctions of Three Patients



The Second Eigenfunction φ_2

(a) $N = 15135$ (b) $N = 15438$ (c) $N = 14938$ (d) $N = 15256$ (e) $N = 14201$ (f) $N = 15630$ (g) $N = 12073$ (h) $N = 12240$

The Third Eigenfunction φ_3

(a) $N = 15135$ (b) $N = 15438$ (c) $N = 14938$ (d) $N = 15256$ (e) $N = 14201$ (f) $N = 15630$ (g) $N = 12073$ (h) $N = 12240$

Classification Results

Dataset consists of the segmented left hippocampuses of 18 DAT subjects and of 26 CN subjects:

Method	Accuracy	Specificity	Sensitivity	n	n'
MomInv	68.1%	69.2%	66.6%	12	1
TensorInv	75.0%	76.9%	72.2%	$\geq 1.9E5$	17
LapEig	77.2%	84.6%	66.6%	998	14
GeodesicInv	86.3%	77.7%	92.3%	$\geq 1.3E6$	27

$$\text{accuracy} := \frac{|TP| + |TN|}{|\text{people examined}|} = \frac{|\text{people correctly diagnosed}|}{|\text{people examined}|}$$

$$\text{specificity} := \frac{|TN|}{|TN| + |FP|} = \frac{|\text{people correctly diagnosed as healthy}|}{|\text{healthy people examined}|}$$

$$\text{sensitivity} := \frac{|TP|}{|TP| + |FN|} = \frac{|\text{people correctly diagnosed as mild AD}|}{|\text{people with mild AD examined}|}$$

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Comparison with PCA

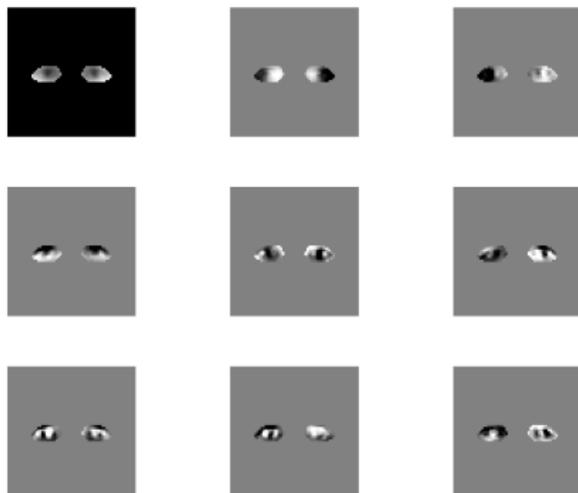
- Consider a stochastic process living on a domain Ω .
- *PCA/Karhunen-Loève Transform* is often used.
- *PCA/KLT implicitly* incorporate geometric information of the measurement (or pixel) location through *data correlation*.
- Our Laplacian eigenfunctions use *explicit* geometric information through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

Comparison with PCA: Example

- “*Rogue’s Gallery*” dataset from Larry Sirovich
- 72 training dataset; 71 test dataset
- Left & right eye regions

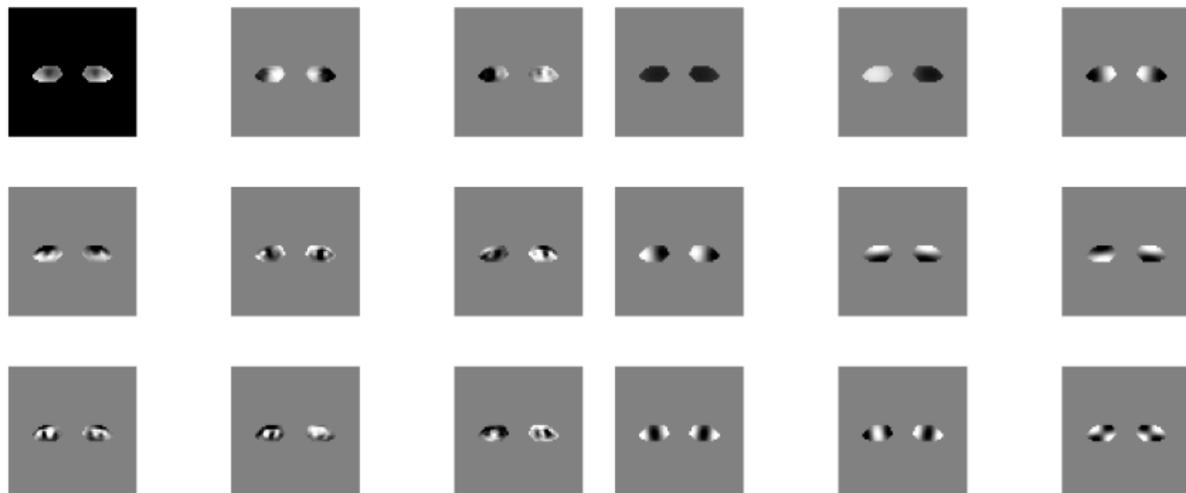


Comparison with PCA: Basis Vectors



(a) KLB/PCA 1:9

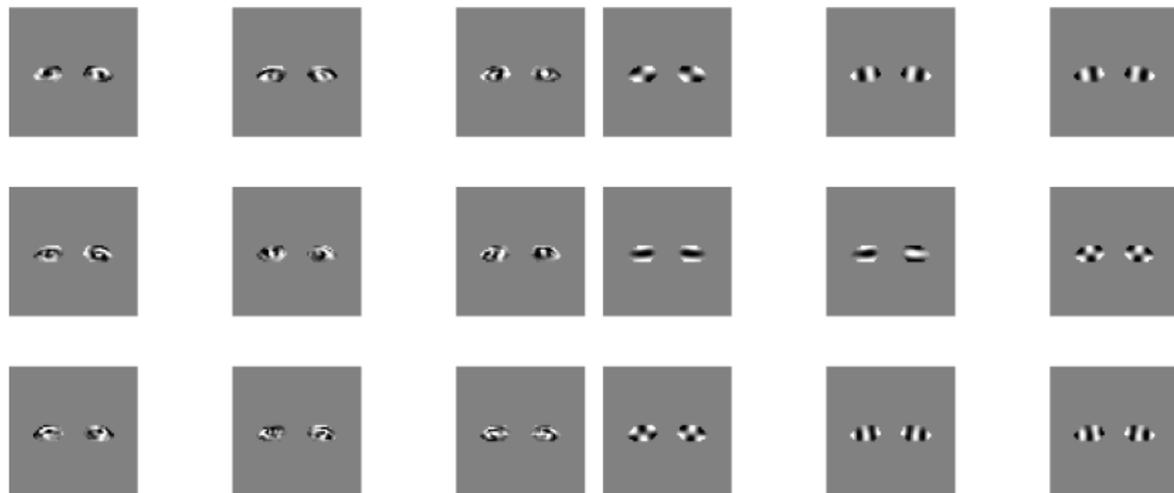
Comparison with PCA: Basis Vectors



(a) KLB/PCA 1:9

(b) Laplacian Eigenfunctions 1:9

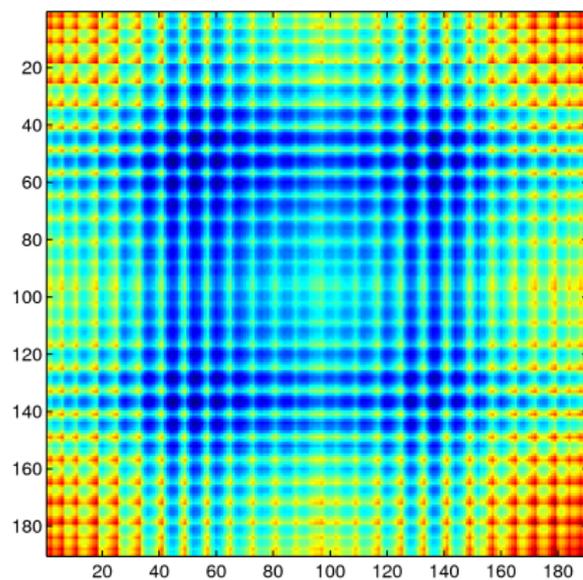
Comparison with PCA: Basis Vectors . . .



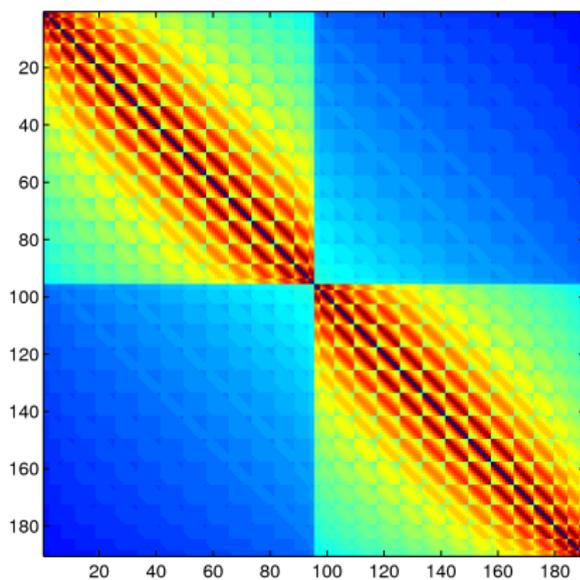
(a) KLB/PCA 10:18

(b) Laplacian Eigenfunctions 10:18

Comparison with PCA: Kernel Matrix

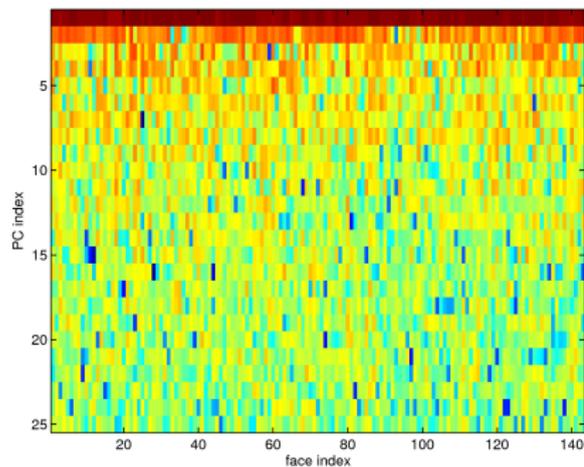


(a) Covariance

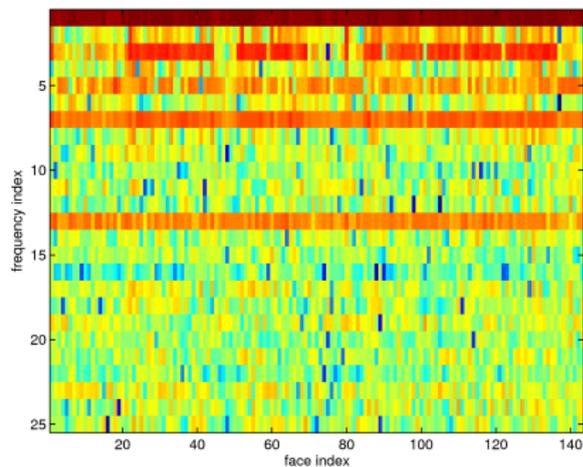


(b) Harmonic kernel

Comparison with PCA: Energy Distribution over Coordinates

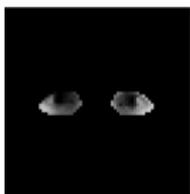


(a) KLB/PCA

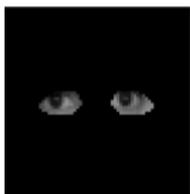


(b) Laplacian Eigenfunctions

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 ...

 $c_{13}:\text{large}$  $c_{13}:\text{large}$  φ_{13}  $c_{13}:\text{small}$  $c_{13}:\text{small}$

Asymmetry Detector



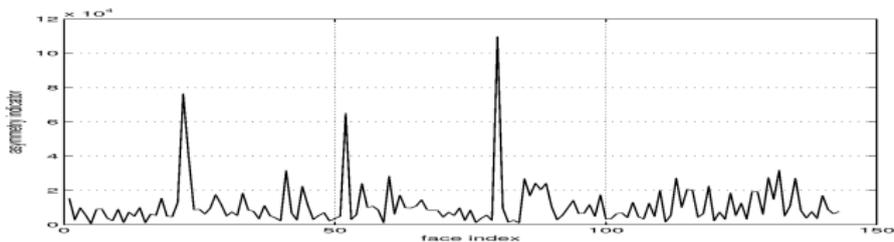
Eyes #80



Eyes #22



Eyes #52



Asymmetry detector



Eyes #5



Eyes #84



Eyes #59

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Summary: Harmonic Analysis of/on Irregular Domains via Laplacian Eigenfunctions

- LEs computed via the commuting integral operator provide an **orthonormal basis** on a general shape domain or a graph and allow **spectral analysis/synthesis** of data on them
- Can get fast-decaying expansion coefficients thanks to the rather implicit BC that may be more natural under certain situations
- Can **decouple geometry** of domains and *statistics* of data
- Can extract **geometric information** of a domain via $\{\lambda_k\}_k$
- Allow **object-oriented** (or localized) data analysis & synthesis, e.g., could be effective for local reconstruction of an ROI and anomaly detection on it
- \exists A variety of applications: interpolation, extrapolation, local feature computation, solving heat equations on complicated domains . . .
- **Fast algorithms** are the key for higher dimensions/large domains
- Can also be defined and computed on a *Riemannian manifold* (e.g., a curved surface); to do so, we need the *Riemannian metric* of the manifold and *geodesic distances* between sample points

References

Laplacian Eigenfunction Resource Page

<http://www.math.ucdavis.edu/~saito/lapeig/> contains:

- My Course Note (elementary) on “Laplacian Eigenfunctions: Theory, Applications, and Computations”
- My Course Slides on “Harmonic Analysis on Graphs and Networks”
- Talk slides of the minisymposia on Laplacian Eigenfunctions at: ICIAM 2007, Zürich (Organizers: NS, Mauro Maggioni); SIAM Imaging Science Conference 2008, San Diego (Organizers: NS, Xiaomin Huo); IPAM 5-day Workshop 2009, UCLA (Organizers: Peter Jones, Denis Grebenkov, NS); SIAM Annual Meeting 2013, San Diego (Organizers: Chiu-Yen Kao, Braxton Osting, NS); BIRS 5-day Workshop 2015, Banff (organizers: Peter Jones, Denis Grebenkov, NS).

The following articles (and the other related ones) are available at <http://www.math.ucdavis.edu/~saito/publications/>

- N. Saito & J.-F. Remy: “The polyharmonic local sine transform: A new tool for local image analysis and synthesis without edge effect,” *Applied & Computational Harmonic Analysis*, vol. 20, no. 1, pp. 41-73, 2006.
- 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.

Thank you very much for your attention!