Laplacian Eigenfunctions That Do Not Feel the Boundary: Theory, Computation, and Applications

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Outline

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Acknowledgment

- Mark Ashbaugh (Univ. Missouri)
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- The MacTutor History of Mathematics Archive, Wikipedia, ...

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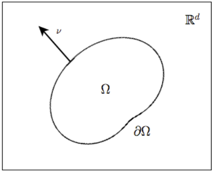
Motivations: Why Irregular/General Shape Domains?

- Consider a bounded domain of general (may be quite complicated) 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 geometric information about the domain $\Omega \Longrightarrow$ shape clustering/classification.



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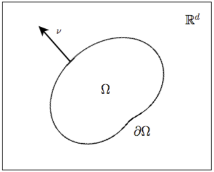

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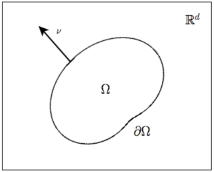

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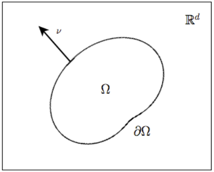

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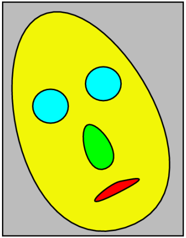
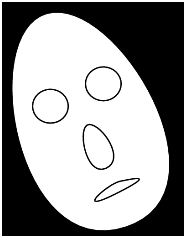
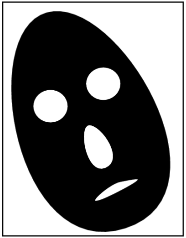
Object-Oriented Image Analysis



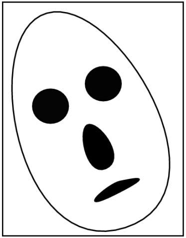
(a) Original



(b) Background

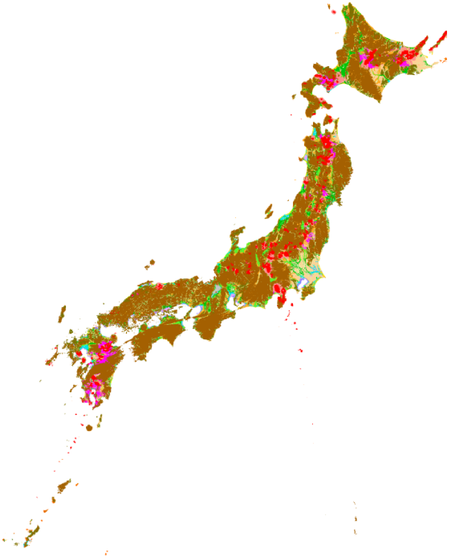


(c) Object

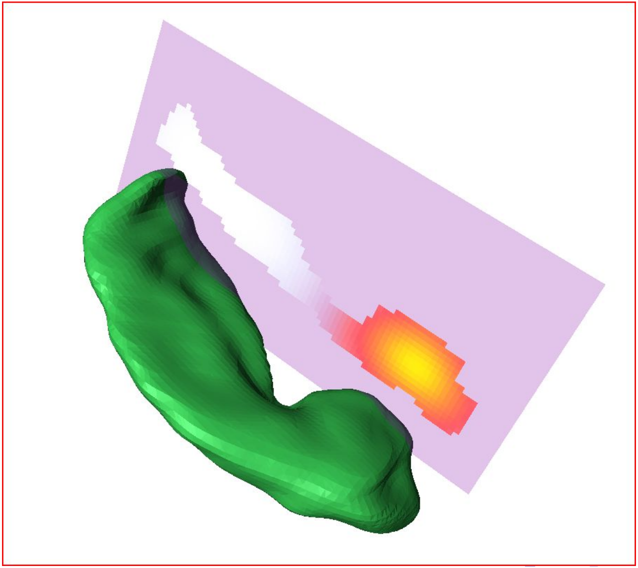


(d) Anomalies

Data Analysis on a Complicated Domain



3D Hippocampus Shape Analysis



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 $\partial\Omega$;
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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: $0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_k \to \infty$.
- On the other hand, the Neumann BC leads to: $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_k \to \infty$.
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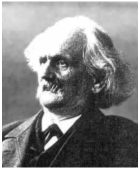
(a) P.-S. Laplace (1749–1827)

(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 $\Longrightarrow$ Generalization of Fourier analysis!

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- 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 $u(x)$, $x \in \Omega$, change over time, i.e., $u(x,t)$, $x \in \Omega$, $t \in [0,T]$. Suppose one want to detect whether there is any change in the material contents in Ω over time, i.e., estimate $u_t(x,t)$ 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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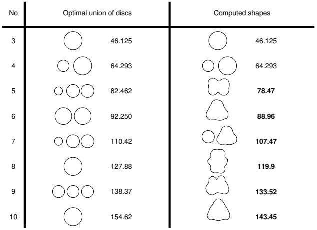
Shape Optimization (Courtesy of B. Osting)

Computational results for single eigenvalues

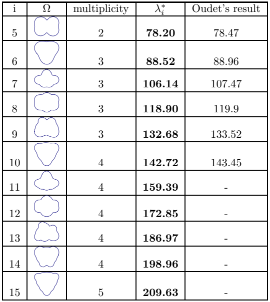
Oudet (2004)



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**

- 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

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**	-

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

Laplacian Eigenfunctions . . . Some Facts

- Analysis of $\mathscr{L}$ 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 $\mathscr{L}^{-1}$ 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 $L^2(\Omega)$.

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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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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

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 $\mathscr{K}\varphi = \mu\varphi$.

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- 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

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

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Integral Operators Commuting with Laplacian . . .

- 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.

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Integral Operators Commuting with Laplacian . . .

- 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:

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

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Integral Operators Commuting with Laplacian ...

Corollary (NS 2009)

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

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

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:

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

Integral Operators Commuting with Laplacian ...

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* $L^2(\Omega)$.

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

1D Example . . .

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

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

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

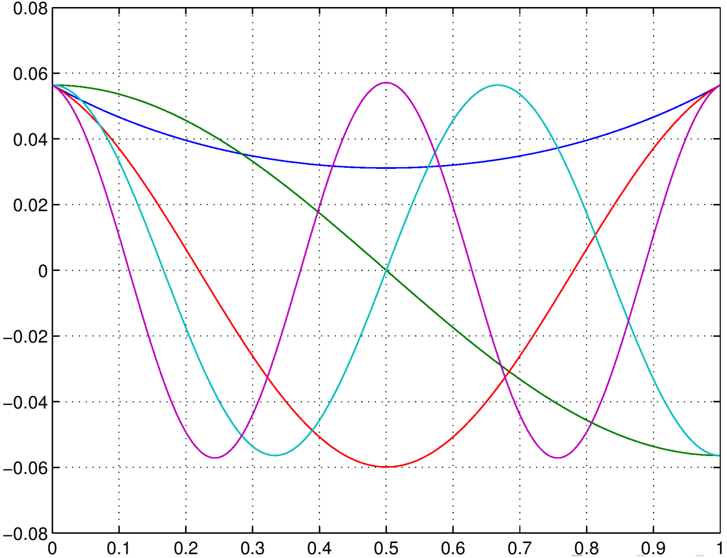
$$\varphi_{2m-1}(x) = \sqrt{2} \cos(2m-1)\pi x;$$

- λ_{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;
Midpoint⇔ DST-II/DCT-II.

1D Example: Rayleigh Functions/Trace Formula

Corollary (NS 2008; See also Hermi & Saito 2013)

Let $\{\lambda_n\}_{n=0}^{\infty}$ be the 1D Laplacian eigenvalues of the non-local boundary problem with the commuting integral operator whose kernel is $K(x,y) = -|x-y|/2$. Then, they satisfy the following trace formula:

$$\sum_{n=0}^{\infty} \frac{1}{\lambda_n} = \int_0^1 K(x,x)\,\mathrm{d}x = 0.$$

Compare this with the famous Basel problem, which is based on the Dirichlet boundary condition:

$$\sum_{n=1}^{\infty} \frac{1}{\pi^2 n^2} = \int_0^1 G_D(x,x)\,\mathrm{d}x = \frac{1}{6} \quad \Longleftrightarrow \quad \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}.$$

1D Example: Rayleigh Functions/Trace Formula ...

Theorem (NS 2008; See also Hermi & Saito 2013)

Let $K_p(x,y)$ be the pth iterated kernel of $K(x,y) = -|x-y|/2$. Then,

$$\sum_{n=0}^{\infty} \frac{1}{\lambda_n^p} = \int_0^1 K_p(x,x)\,\mathrm{d}x = \frac{1}{4^p}\left(S_{2p} + \frac{(-1)^p}{\alpha^{2p}}\right) + \frac{4^p - 1}{2 \cdot (2p)!}|B_{2p}|,$$

where $\alpha \approx 1.19967864$ satisfies $\alpha = \coth\alpha$, B_{2p} is the Bernoulli number, and

$$S_{2p} := \sum_{m=1}^{\infty} \left(\frac{4}{\lambda_{2m}}\right)^p,$$

satisfies the following recursion formula:

$$\sum_{\ell=1}^{n+1} \frac{(-1)^{n-\ell+1}(2(n-\ell+1)-1)}{(2(n-\ell+1))!}\left\{S_{2\ell} + \frac{(-1)^\ell}{\alpha^{2\ell}}\right\} = \frac{(-1)^n}{2(2n)!}.$$

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.,

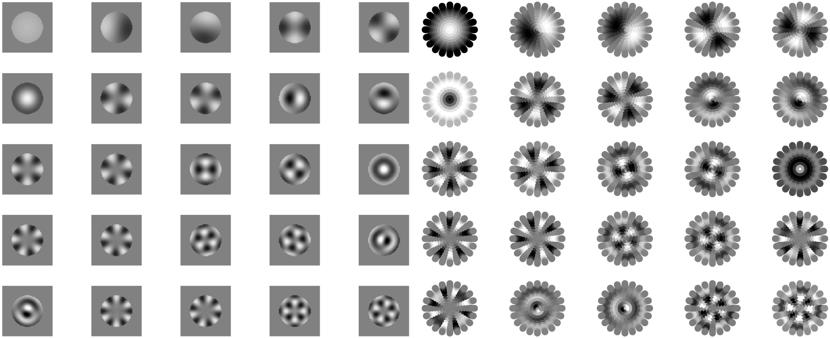
$$\mathscr{H}f(\theta) := \frac{1}{2\pi}\,\mathrm{pv}\!\int_{-\pi}^{\pi} f(\eta)\cot\left(\frac{\theta-\eta}{2}\right)\mathrm{d}\eta \quad \theta\in[-\pi,\pi].$$

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

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

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

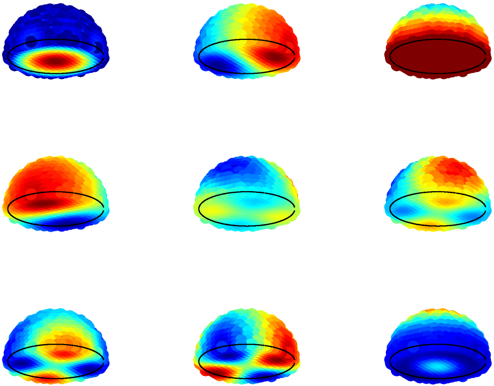
First 25 Basis Functions



(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

Connection with Potential Theory

- Mark Kac mentioned at the very end of his 1951 paper (Proceedings of the 2nd Berkeley Symposium on Mathematical Statistics and Probability) that the same integral equation in 3D is equivalent to the Laplacian eigenvalue problem. But his BC was incorrect.
- In 1967–9, John Troutman studied the eigenvalues of the same integral operator (i.e., the logarithmic potential) in 2D. He posed this problem as the Laplacian eigenvalue problem whose eigenfunctions are harmonic outside of the given domain. He proved that there exists one negative eigenvalue iff the *transfinite diameter* (or *logarithmic capacity*) of the closed domain $\overline{\Omega}$ exceeds 1.
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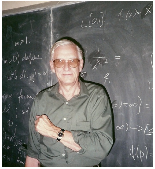
(a) Mark Kac (1914–1984)



(b) John Troutman (193?–)

(c) Tomasz Bojdecki (?)

Connection with Volterra Operators

- The 1959 paper of Victor B. Lidskiĭ "Conditions for completeness of a system of root subspaces for non-selfadjoint operators with discrete spectra," *Amer. Math. Soc. Transl. Ser. 2*, vol. 34, pp. 241–281, 1963, discusses the *iterated Volterra integral operator*:

$$Af(x) := \int_x^1 f(y)\,\mathrm{d}y,\ f \in L^2(0,1) \Longrightarrow A^2 f(x) = \int_x^1 (x-y) f(y)\,\mathrm{d}y$$

which was decomposed into the real and imaginary parts:

$$\begin{aligned} (A^2)_R f &:= \frac{1}{2}(A^2 + A^{2*}) = -\frac{1}{2}\int_0^1 |x-y| f(y)\,\mathrm{d}y; \\ (A^2)_I f &:= \frac{1}{2\mathrm{i}}(A^2 - A^{2*}) = \frac{1}{2\mathrm{i}}\int_0^1 (x-y) f(y)\,\mathrm{d}y. \end{aligned}$$

Connection with Volterra Operators . . .

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- Do the higher dimensional cases have also similar correspondence?

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(a) Victor Lidskiĭ (1924–2008)

(b) Mark Krein (1907–1989)

(c) Israel Gohberg (1928–2009)

Connection with von Neumann–Kreĭn Extension Theory

- John von Neumann (1929) and Mark Kreĭn (1947) considered a *self-adjoint extension of symmetric operators*.
- Let $T := -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$, $\mathscr{D}(T) := H_0^2(0,1) \subset H^2(0,1)$, where $H_0^2(0,1) := \{f \in H^2(0,1) \mid f(0) = f(1) = f'(0) = f'(1) = 0\}$ and $H^2(0,1) := \{f \in C^1[0,1] \mid f' \in AC[0,1], f'' \in L^2(0,1)\}$. T is a positive *symmetric* operator on $\mathscr{D}(T)$, but *not self-adjoint* because $\mathscr{D}(T^*) = H^2(0,1) \supsetneq \mathscr{D}(T)$.
- von Neumann-Kreĭn extension of T is the smallest (or soft) self-adjoint extension $T_0 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$, $\mathscr{D}(T_0) = \{f \in H^2(0,1) \mid f'(0) = f'(1) = f(1) - f(0)\} = \mathscr{D}(T_0^*)$.

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Connection with von Neumann–Kreĭn Extension Theory . . .

- Compare it with our boundary condition: $-f'(0) = f'(1) = f(0) + f(1)$.
- Also, compare it with the *Friedrichs extension* of T, which is the *largest (or hard) self-adjoint extension*: $T_\infty = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$, $\mathscr{D}(T_\infty) = \left\{ f \in H^2(0,1) \mid f(0) = f(1) = 0 \right\} = \mathscr{D}(T_\infty^*) \Longleftrightarrow$ Dirichlet BC!

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(a) John von Neumann (1903–1957)

(b) Mark Krein (1907–1989)

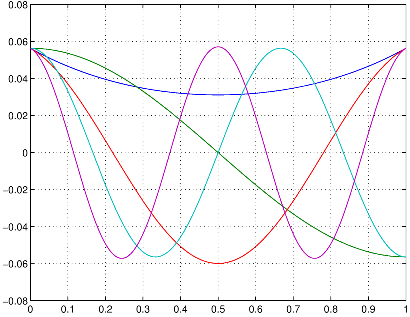
(c) Kurt Friedrichs (1901–1982)

Connection with von Neumann–Kreĭn Extension Theory . . .

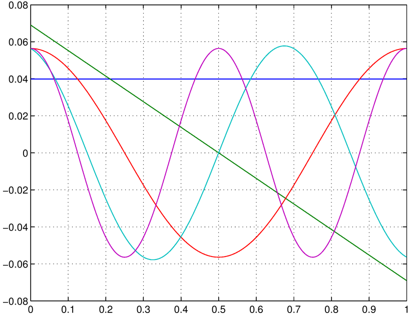
	Our Basis	Kreĭn-Laplacian Basis
λ_0	-5.756915. . . ; $\tanh \sqrt{-\lambda_0}/2 = 2/\sqrt{-\lambda_0}$	0
φ_0	$\cosh \sqrt{-\lambda_0}(x-1/2)$	1
λ_1	π^2	0
φ_1	$\sin \pi(x-1/2)$	1/2-x
λ_{2m}	$\tan \sqrt{\lambda_{2m}}/2 = -2/\sqrt{\lambda_{2m}}$	$(2m\pi)^2$
φ_{2m}	$\cos \sqrt{\lambda_{2m}}(x-1/2)$	$\cos 2m\pi(x-1/2)$
λ_{2m+1}	$((2m+1)\pi)^2$	$\tan \sqrt{\lambda_{2m+1}}/2 = \sqrt{\lambda_{2m+1}}/2$
φ_{2m+1}	$\sin(2m+1)\pi(x-1/2)$	$\sin \sqrt{\lambda_{2m+1}}(x-1/2)$

Note that the above eigenfunctions are not normalized to have $\|\cdot\|_2 = 1$.

Connection with von Neumann–Kreĭn Extension Theory . . .



(a) Our Basis



(b) Kreĭn-Laplacian Basis

Connection with von Neumann–Kreĭn Extension Theory ...

- In higher dimensions, the von Neumann-Kreĭn extension of the Laplacian $T = -\Delta$, $\mathscr{D}(T) = H_0^2(\Omega)$, on $\Omega \subset \mathbb{R}^d$ turns out to be: $T_0 = -\Delta$, $\mathscr{D}(T_0) = \left\{ f \in H^2(\Omega) \,\middle|\, \frac{\partial f}{\partial \nu}(\boldsymbol{x}) = \frac{\partial H(f)}{\partial \nu}(\boldsymbol{x}), \boldsymbol{x} \in \partial\Omega \right\}$ where $H(f)$ is a harmonic function in Ω with the boundary condition: $H(f) = f$ on $\partial\Omega$; See e.g., A. Alonso & B. Simon: "The Birman-Kreĭn-Vishik theory of self-adjoint extensions of semibounded operators," *J. Operator Theory*, vol. 4, pp. 251–270, 1980.
- This is closely related to our Polyharmonic Local Sine Transform (PHLST): N. Saito & J.-F. Remy: "The polyharmonic local sine transform: A new tool for local image analysis and synthesis without edge effect," *Appl. Comput. Harm. Anal.*, vol. 20, pp. 41–73, 2006.
- After all, the von Neumann-Kreĭn extensions do not deal with the exterior of the domain Ω while our approach based on the commuting integral operators allow us to extend our eigenfunctions very naturally to the exterior of Ω.

Connection with von Neumann–Kreĭn Extension Theory . . .

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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 $\boldsymbol{\varphi} := (\varphi_1, \ldots, \varphi_N)^T \in \mathbb{R}^N$. 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

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.
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Outline

Incorporating 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 $\boldsymbol{\chi}_\Omega := \mathbf{1}_N/\sqrt{N} \in \mathbb{R}^N$.
- 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 $\operatorname{span}\{\chi_\Omega\}$ in the column space of the kernel matrix K:

$$\widetilde{K} = \left(I - \chi_\Omega \chi_\Omega^\top\right) K.$$

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

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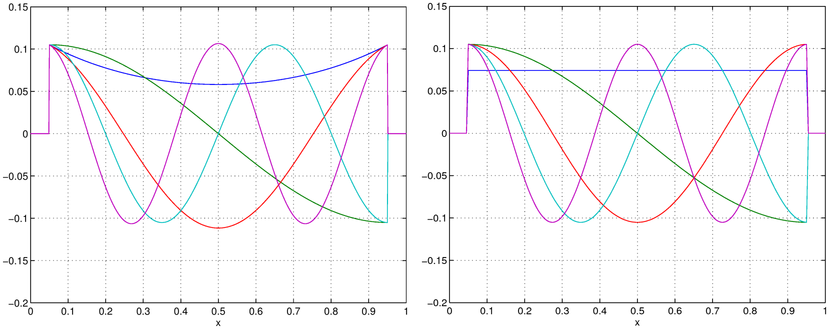
Incorporating the DC vector ...



(a) Laplacian Eigenfunctions via Commuting Integral Operator

(b) Laplacian Eigenfunctions incorporating the DC vector

$\Longrightarrow$ leads to the *generalized discrete cosine basis!*

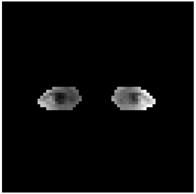
Outline

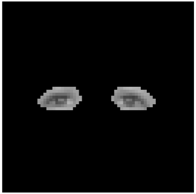
Comparison with PCA

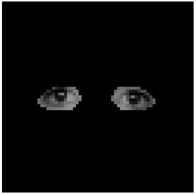
- Consider a stochastic process living on a domain Ω.
- *PCA/Karhunen-Loève Transform* is often used.
- PCA/KLT *implicitly* incorporate geometric information of the measurement (or pixel) location through *data correlation*.
- Our Laplacian eigenfunctions use *explicit* geometric information through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

Comparison with PCA: Example

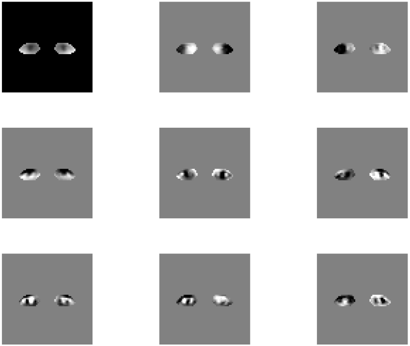
- *"Rogue's Gallery"* dataset from Larry Sirovich
- 72 training dataset; 71 test dataset
- Left & right eye regions







Comparison with PCA: Basis Vectors



(a) KLB/PCA 1:9

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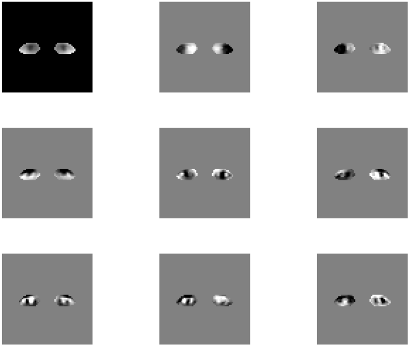

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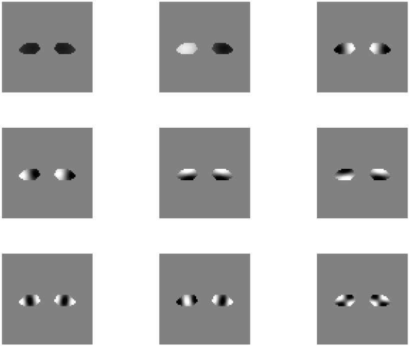
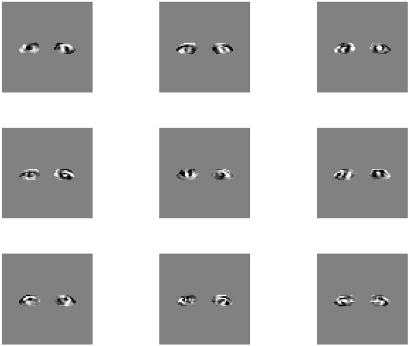
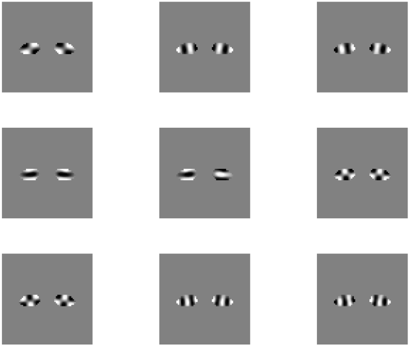


(b) Laplacian Eigenfunctions 1:9

Comparison with PCA: Basis Vectors . . .

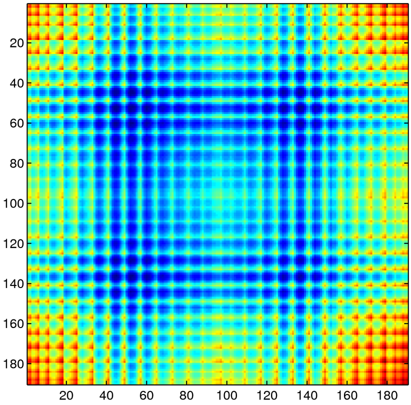


(a) KLB/PCA 10:18

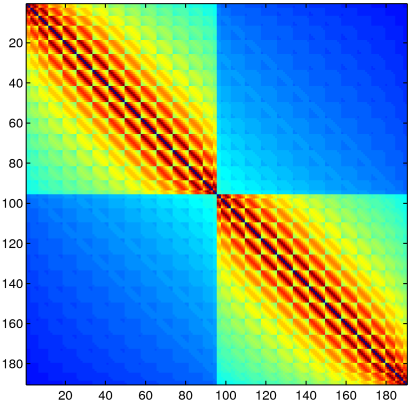


(b) Laplacian Eigenfunctions 10:18

Comparison with PCA: Kernel Matrix

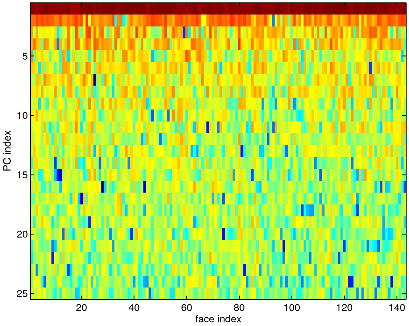


(a) Covariance

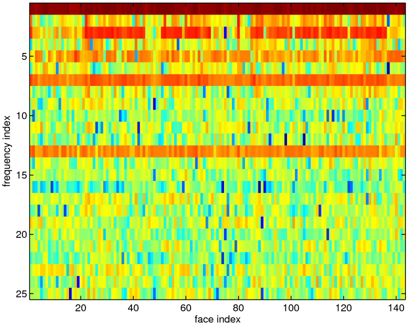


(b) Harmonic kernel

Comparison with PCA: Energy Distribution over Coordinates

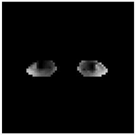


(a) KLB/PCA

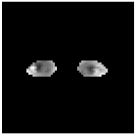


(b) Laplacian Eigenfunctions

Comparison with PCA: Basis Vector #7 . . .

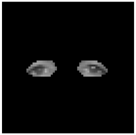


c_7:large

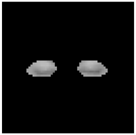


c_7:large

φ_7

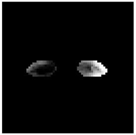


c_7:small

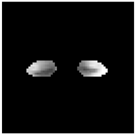


c_7:small

Comparison with PCA: Basis Vector #13 . . .



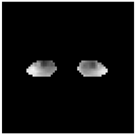
c_{13}:large



c_{13}:large

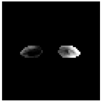
φ_{13}

c_{13}:small

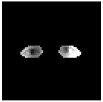


c_{13}:small

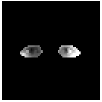
Asymmetry Detector



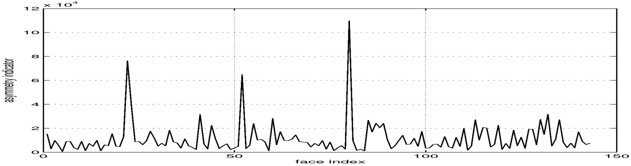
Eyes #80



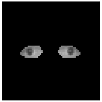
Eyes #22



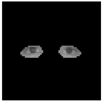
Eyes #52



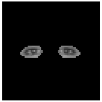
Asymmetry detector



Eyes #5

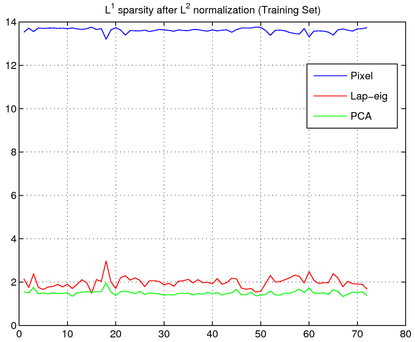


Eyes #84



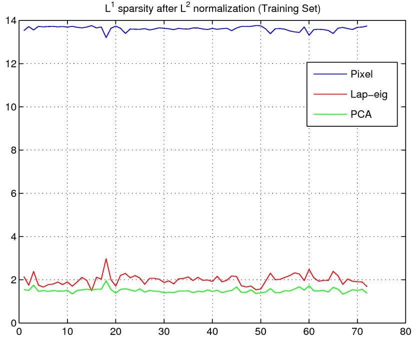
Eyes #59

Comparison with PCA: Sparsity



(a) Training set

Comparison with PCA: Sparsity



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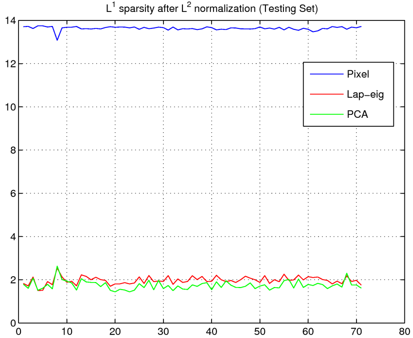
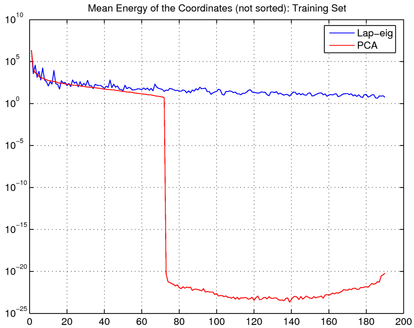


(b) Test set

Comparison with PCA: Coefficient Decay



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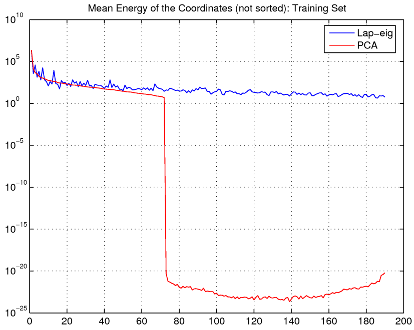

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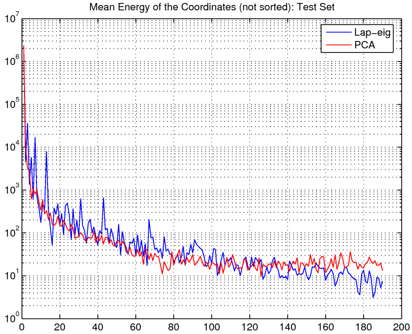


(b) Test set

Outline

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

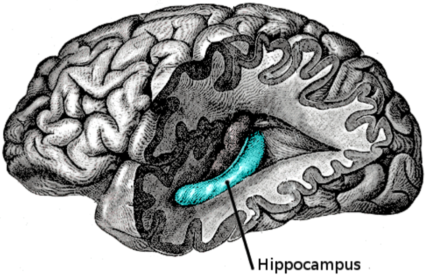


Figure: From Wikipedia

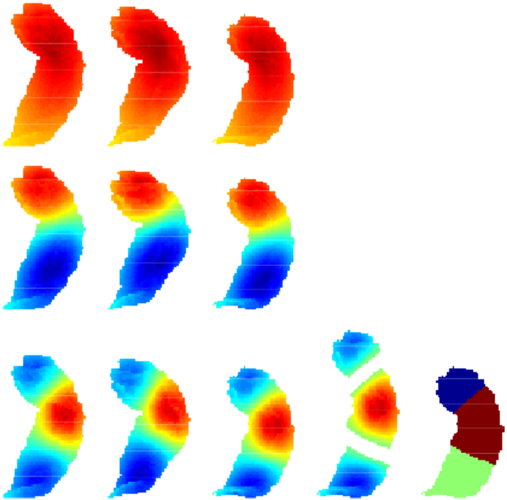
Hippocampal Shape Analysis . . .

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

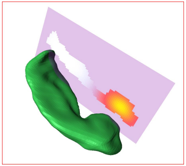
$$\boldsymbol{F} := \left(\frac{\lambda_1}{\lambda_2}, \dots, \frac{\lambda_1}{\lambda_{n+1}}\right)^{\mathsf{T}} = \left(\frac{\mu_2}{\mu_1}, \dots, \frac{\mu_{n+1}}{\mu_1}\right)^{\mathsf{T}} \in \mathbb{R}^n.$$

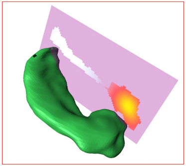
  This feature vector was used by Khabou, Hermi, and Rhouma (2007) for 2D shape classification (e.g., shapes of tree leaves).
- Reduce the feature space dimension via PCA to from $n = 998$ to n'
- Classified by the linear SVM (support vector machine)

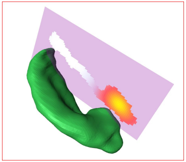
First Three Eigenfunctions of Three Patients

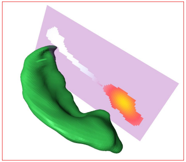


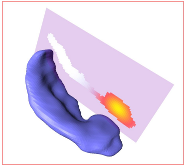
The Second Eigenfunction φ_2

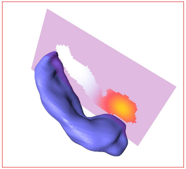

(a) $N = 15135$

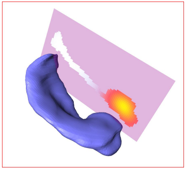

(b) $N = 15438$

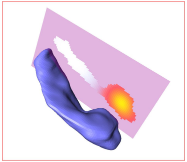

(c) $N = 14938$


(d) $N = 15256$

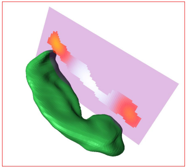

(e) $N = 14201$


(f) $N = 15630$

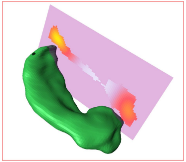

(g) $N = 12073$


(h) $N = 12240$

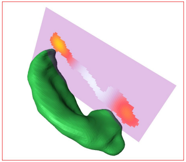
The Third Eigenfunction φ_3



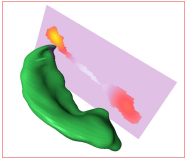
(a) $N = 15135$



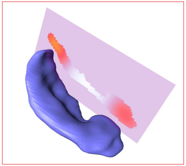
(b) $N = 15438$



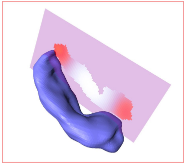
(c) $N = 14938$



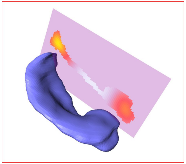
(d) $N = 15256$



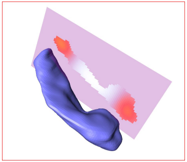
(e) $N = 14201$



(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

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

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

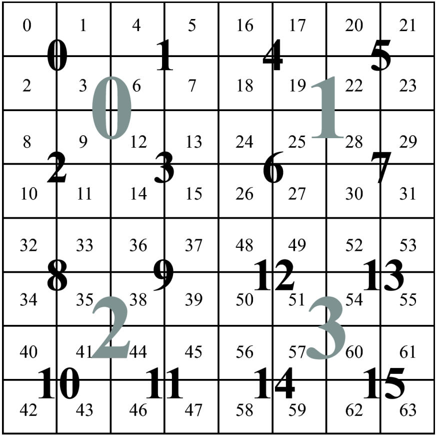
$$\text{sensitivity} := \frac{|TP|}{|TP| + |FN|} = \frac{|\text{people correctly diagnosed as mild AD}|}{|\text{people with mild AD examined}|}$$

Outline

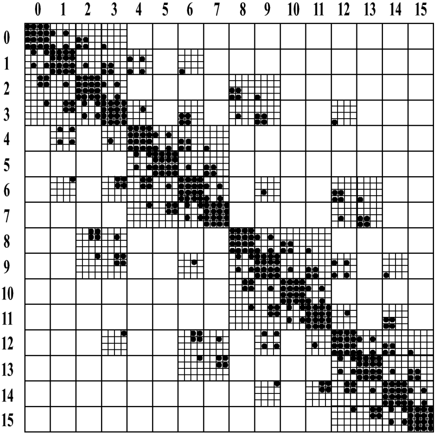
A Possible Fast Algorithm for Computing φ_j's

- 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

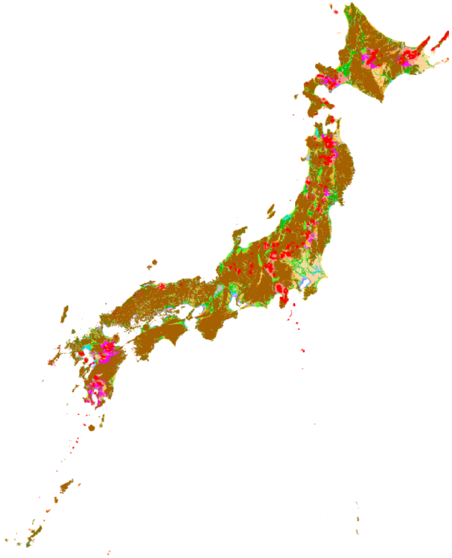


(a) Hierarchical indexing scheme

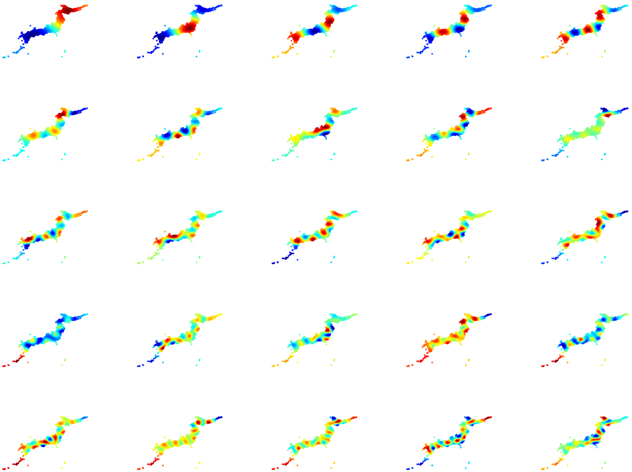


(b) Tree-Structured Matrix

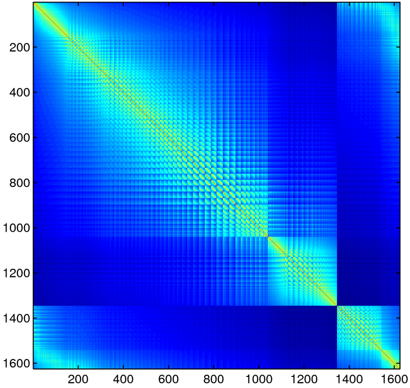
A Real Challenge: Kernel matrix is of 387924×387924.



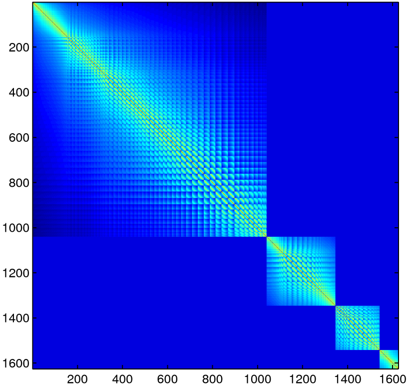
First 25 Basis Functions via the FMM-based algorithm



Splitting into Subproblems for Faster Computation

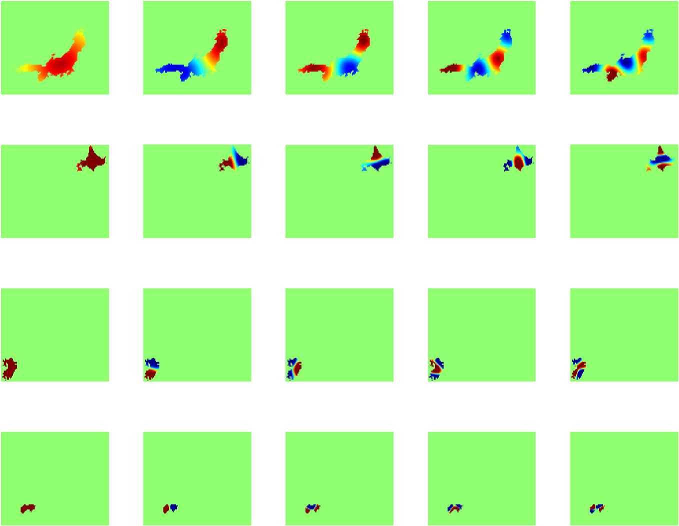


(a) Whole islands



(b) Separated islands

Eigenfunctions for Separated Islands



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
- Many things to be done:
  - Examine further our boundary conditions for specific geometry in higher dimensions; e.g., analysis of $\mathbb{S}^2$ leads to *Clifford Analysis*
  - Examine the relationship with the *Volterra operators* in $\mathbb{R}^d$, $d \geq 2$ (Lidskiĭ; Gohberg-Kreĭn)
  - Integral operators commuting with polyharmonic operators $(-\Delta)^p$, $p \geq 2$?

Outline

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 & 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.
  - L. Hermi & N. Saito: "On Rayleigh-type formulas for a non-local boundary value problem associated with an integral operator commuting with the Laplacian," preprint, 2014.

Thank you very much for your attention!