

# Use of Laplacian Eigenfunctions and Eigenvalues for Analyzing Data on a Domain of Complicated Shape

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# Outline

- 1 Motivations
- 2 Laplacian Eigenfunctions
- 3 Integral Operators Commuting with Laplacian
- 4 Examples
  - 1D Example
  - 2D Example
  - 3D Example
- 5 Discretization of the Problem
- 6 Applications
  - Image Approximation
  - Statistical Image Analysis; Comparison with PCA
  - Solving the Heat Equation on a Complicated Domain
  - Clustering Mouse Retinal Ganglion Cells
- 7 Fast Algorithms for Computing Eigenfunctions
- 8 Conclusions

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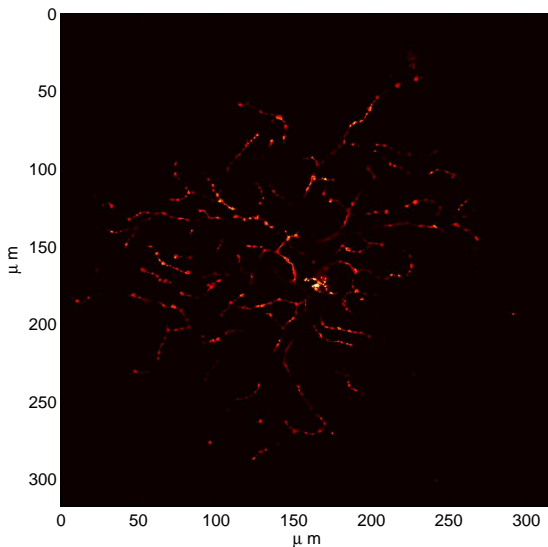
# Motivations

- 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  $\Omega \implies$  need to avoid **the Gibbs phenomenon** due to  $\Gamma = \partial\Omega$ .
- Want to represent the object information efficiently for analysis, interpretation, discrimination, etc.  $\implies$  **fast decaying** expansion coefficients relative to a **meaningful** basis.
- Want to extract **geometric information** about the domain  $\Omega \implies$  shape clustering/classification.

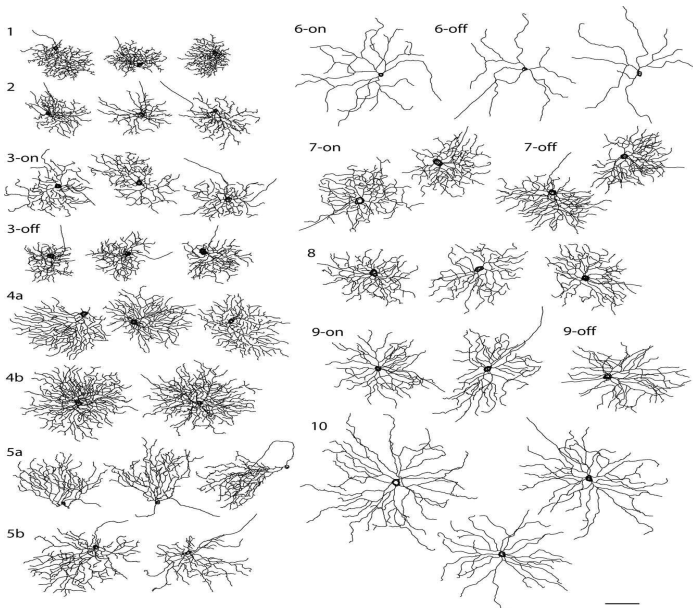
# Motivations . . . Data Analysis on a Complicated Domain



# Motivations ... Clustering Complicated Objects



# Motivations ... Clustering Complicated Objects ...



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# Eigenfunctions of Laplacian

- Our previous attempt was to extend the object to the outside smoothly and then bound it nicely with a rectangular box followed by the ordinary Fourier analysis.
- Why not analyze (and synthesize) the object using **genuine basis functions tailored to the domain?**
- After all, *sines* (and *cosines*) are the eigenfunctions of the Laplacian on the *rectangular* domain 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.

# Eigenfunctions of Laplacian ...

- Consider an operator  $\mathcal{L} = -\Delta$  in  $L^2(\Omega)$  with *appropriate* boundary condition.
- Analysis of  $\mathcal{L}$  is difficult due to 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  $L^2(\Omega)$ .

- The key difficulty is to compute such eigenfunctions; directly solving the Helmholtz equation (or eigenvalue problem) on a general domain is tough.
- Unfortunately, computing the Green's function for a general  $\Omega$  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 is to find an integral operator **commuting** with the Laplacian without imposing the strict boundary condition a priori.
- Then, we know that the eigenfunctions of the Laplacian is the same as those of the integral operator, which is easier to deal with, due to the following

Theorem (G. Frobenius 1878?; 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  $\mathcal{K}\varphi = \mu\varphi$ .*

- Let's replace the Green's function  $G(\mathbf{x}, \mathbf{y})$  by the **fundamental solution of the Laplacian**:

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

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

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

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

## Theorem (NS 2005)

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

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

for all  $\mathbf{x} \in \Gamma$ , where  $\varphi$  is an eigenfunction common for both operators.

## Corollary (NS 2005)

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

# 1D Example ...

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

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

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

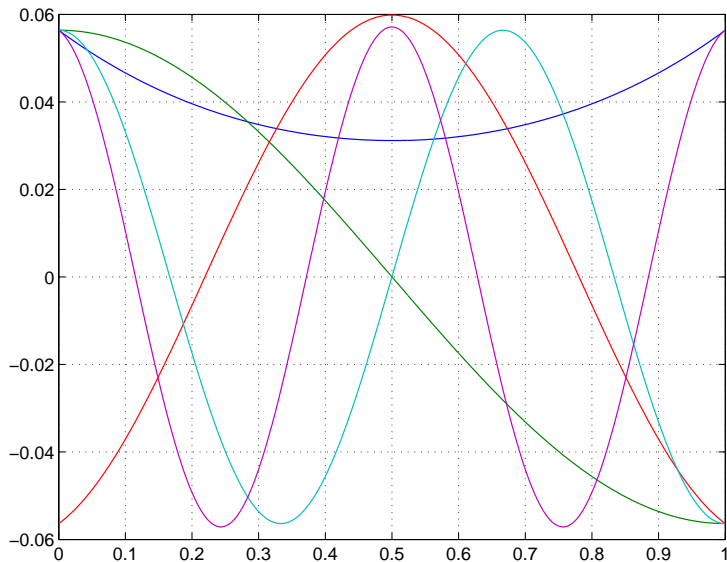
$$\varphi_{2m-1}(x) = \sqrt{2} \cos(2m-1)\pi x;$$

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

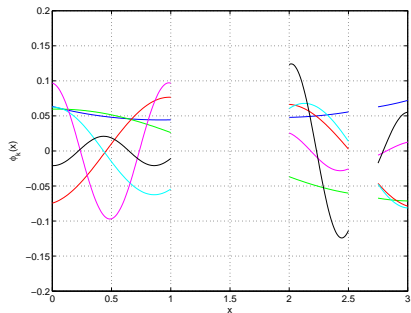
$$\varphi_{2m}(x) = A_{2m} \cos \sqrt{\lambda_{2m}} \left( x - \frac{1}{2} \right),$$

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

# First 5 Basis Functions

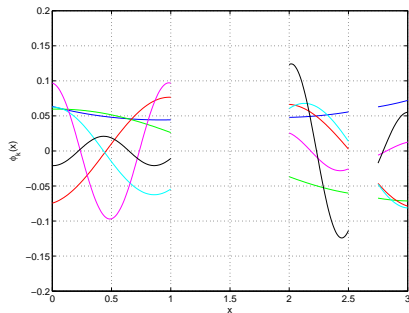


# 1D Example: Bases on Disconnected Intervals

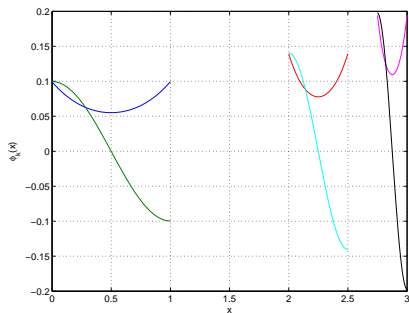


(a) Union

# 1D Example: Bases on Disconnected Intervals



(a) Union



(b) Separated

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## 2D Example

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

$$-\Delta\varphi = \lambda\varphi, \quad \text{in } \Omega;$$
$$\frac{\partial\varphi}{\partial\nu}\Big|_{\Gamma} = \frac{\partial\varphi}{\partial r}\Big|_{\Gamma} = -\frac{\partial\mathcal{H}\varphi}{\partial\theta}\Big|_{\Gamma},$$

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

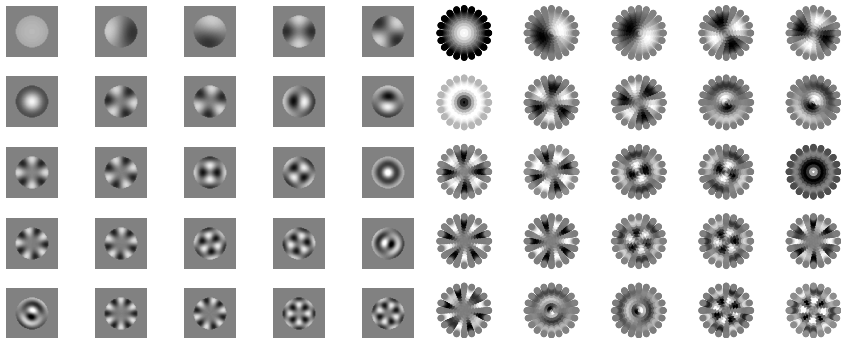
$$\mathcal{H}f(\theta) \triangleq \frac{1}{2\pi} \text{pv} \int_{-\pi}^{\pi} f(\eta) \cot\left(\frac{\theta - \eta}{2}\right) d\eta \quad \theta \in [-\pi, \pi].$$

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

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

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

# First 25 Basis Functions



(a) Our Basis

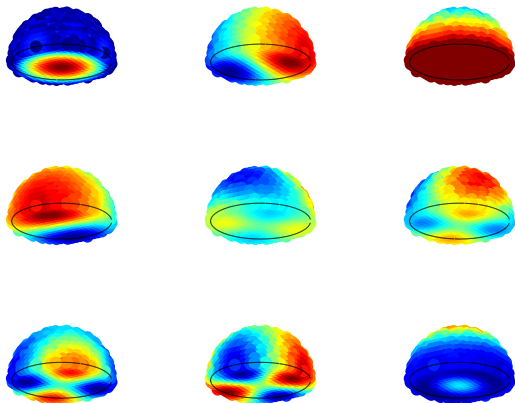
(b) Dirichlet-Laplace

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# 3D Example

- Consider the unit ball  $\Omega$  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  $\Omega$  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  $K_{i,j} \triangleq w_j K(\mathbf{x}_i, \mathbf{x}_j)$ ,  $\varphi_i \triangleq \varphi(\mathbf{x}_i)$ , and  $\boldsymbol{\varphi} \triangleq (\varphi_1, \dots, \varphi_N)^T \in \mathbb{R}^N$ . 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**.

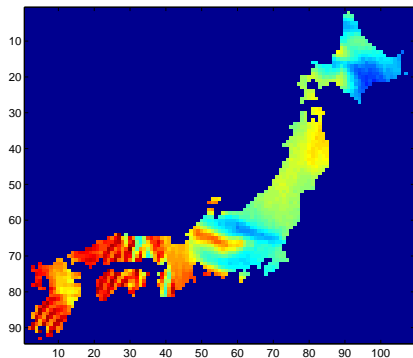
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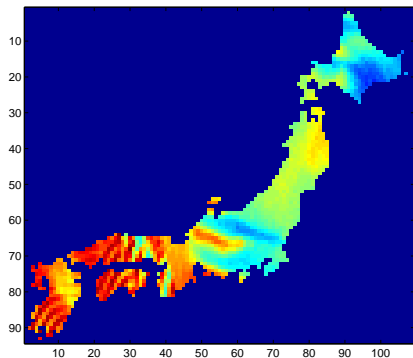
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# Image Approximation; Comparison with Wavelets

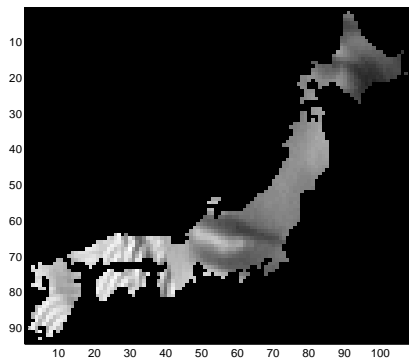


(a) What data?

# Image Approximation; Comparison with Wavelets

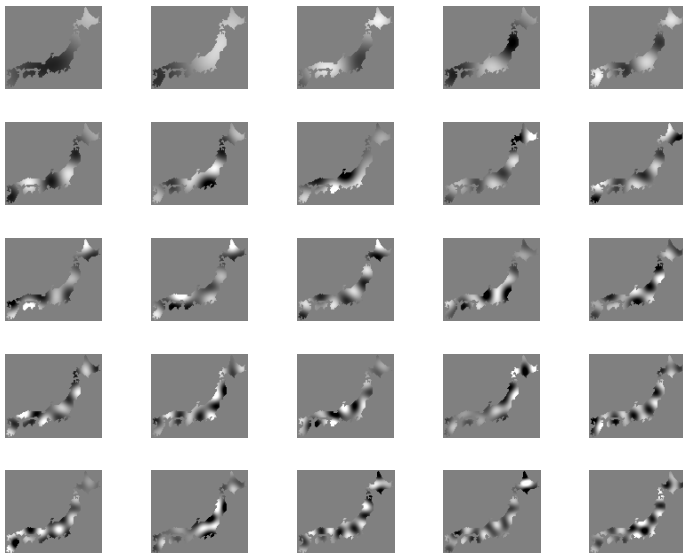


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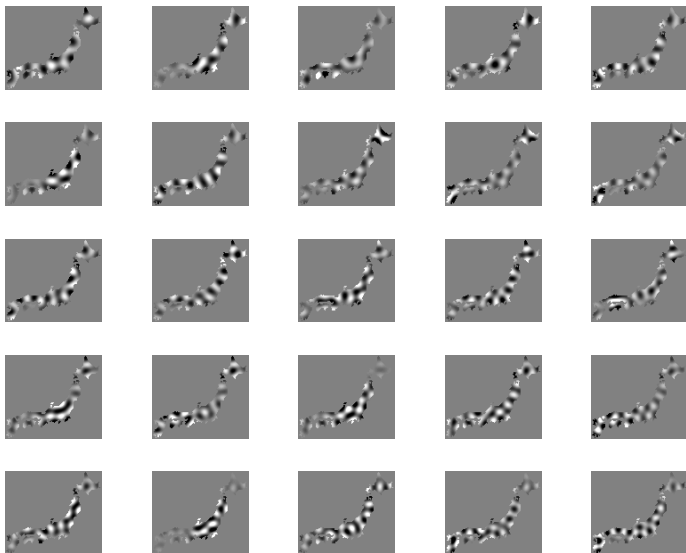


(b)  $\chi_J$ : Barbara

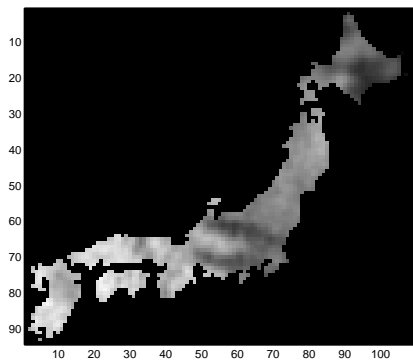
# First 25 Basis Functions



# Next 25 Basis Functions

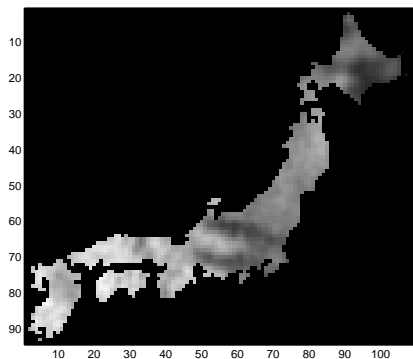


# Reconstruction with Top 100 Coefficients

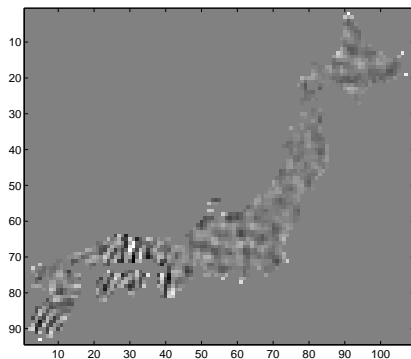


(a) Reconstruction

# Reconstruction with Top 100 Coefficients

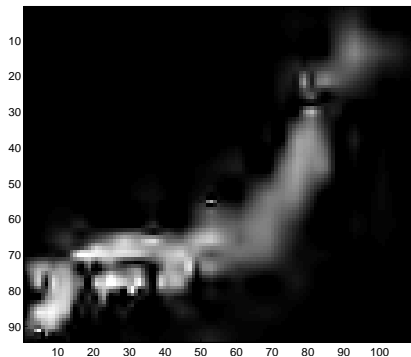


(a) Reconstruction



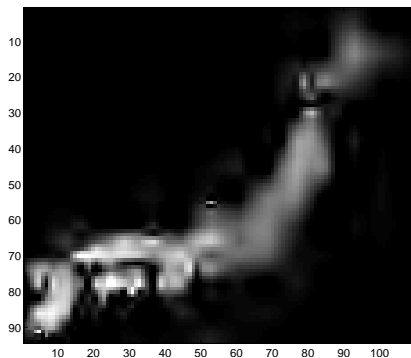
(b) Error

# Reconstruction with Top 100 2D Wavelets (Symmlet 8)

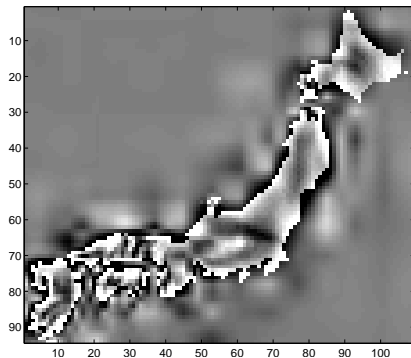


(a) Reconstruction

# Reconstruction with Top 100 2D Wavelets (Symmlet 8)

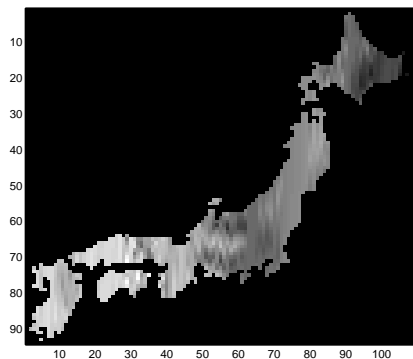


(a) Reconstruction



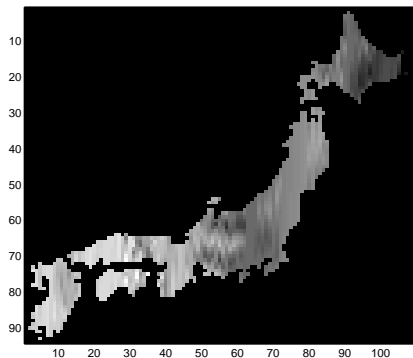
(b) Error

# Reconstruction with Top 100 1D Wavelets (Symmlet 8)

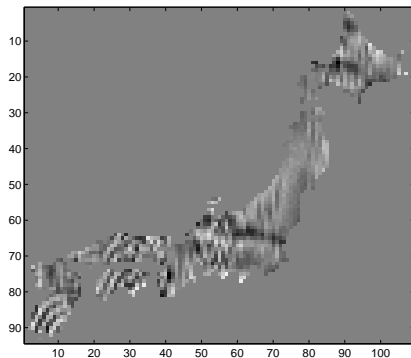


(a) Reconstruction

# Reconstruction with Top 100 1D Wavelets (Symmlet 8)

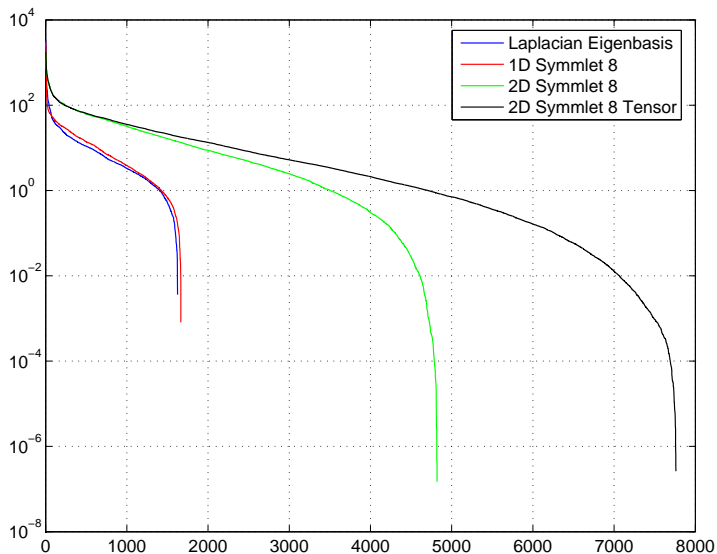


(a) Reconstruction



(b) Error

# Comparison of Coefficient Decay



A Real Challenge: Kernel matrix is of  $387924 \times 387924$ .



# Conjecture on the Coefficient Decay Rate

## Conjecture (NS 2005)

*For  $f \in C(\overline{\Omega})$  with  $\nabla f \in BV(\overline{\Omega})$  defined on  $C^2$ -domain  $\Omega$ , the expansion coefficients  $\langle f, \varphi_k \rangle$  w.r.t. the Laplacian eigenbasis decay as  $O(k^{-2})$ . Thus, the  $N$ -term approximation error measured in the  $L^2$ -norm should have a decay rate of  $O(N^{-1.5})$ .*

# Outline

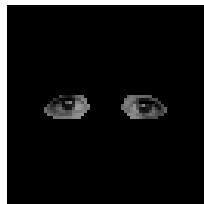
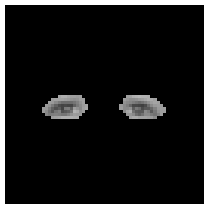
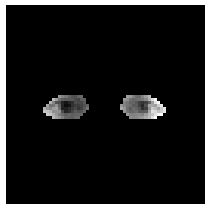
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# Comparison with PCA

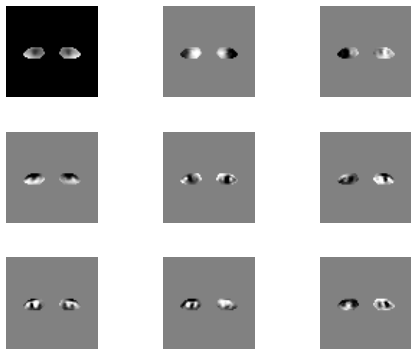
- Consider a stochastic process living on a domain  $\Omega$ .
- PCA/Karhunen-Loève Transform is often used.
- PCA/KLT incorporate geometric information of the measurement (or pixel) location through the data correlation, i.e., implicitly.
- Our Laplacian eigenfunctions use explicit geometric information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

# Comparison with PCA: Example

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

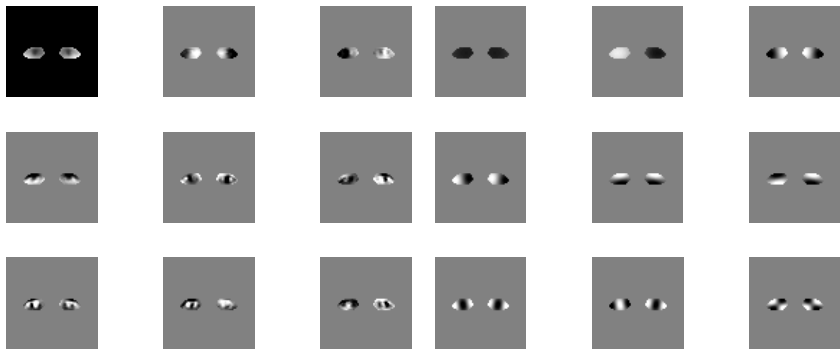


# Comparison with PCA: Basis Vectors



(a) KLB/PCA 1:9

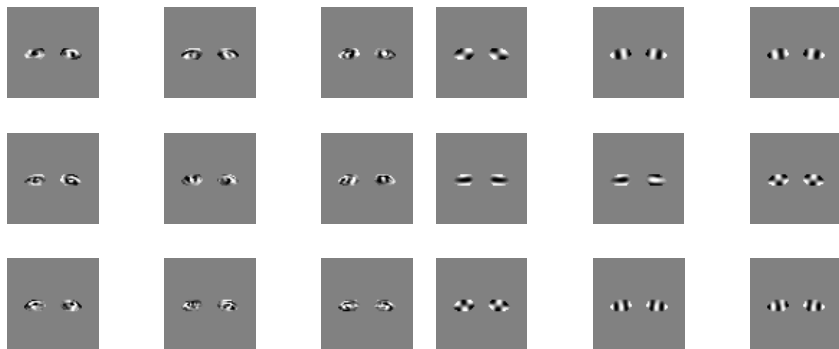
# Comparison with PCA: Basis Vectors



(a) KLB/PCA 1:9

(b) Laplacian Eigenfunctions 1:9

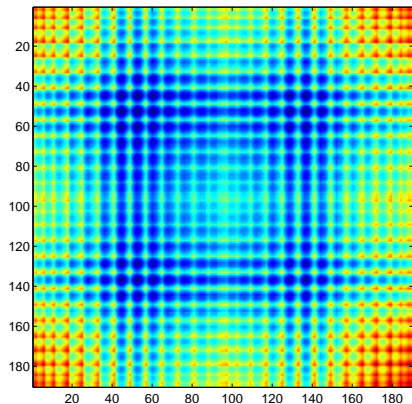
# Comparison with PCA: Basis Vectors ...



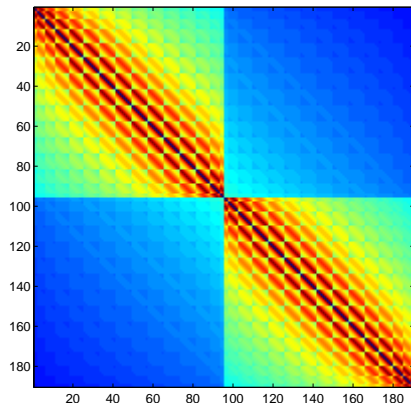
(a) KLB/PCA 10:18

(b) Laplacian Eigenfunctions 10:18

# Comparison with PCA: Kernel Matrix

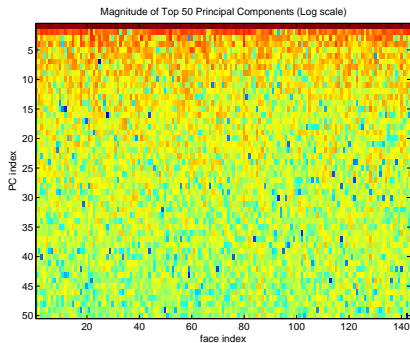


(a) Covariance

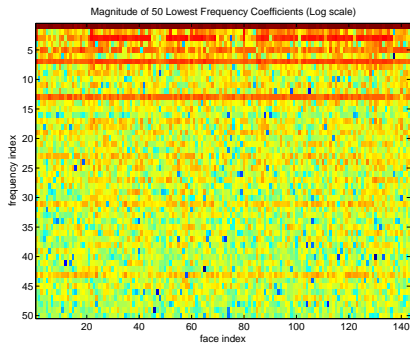


(b) Harmonic kernel

# Comparison with PCA: Energy Distribution over Coordinates

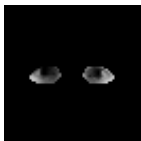


(a) KLB/PCA



(b) Laplacian Eigenfunctions

# Comparison with PCA: Basis Vector #7 ...



$c_7$ :large



$c_7$ :large



$\varphi_7$

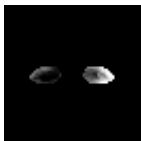


$c_7$ :small



$c_7$ :small

# Comparison with PCA: Basis Vector #13 ...



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



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



$\varphi_{13}$



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



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

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# Solving the Heat Equation on a Complicated Domain

- It is well known that the semigroup  $e^{t\Delta}$  can be diagonalized using the Laplacian eigenbasis, i.e., for any initial heat distribution  $u_0(\mathbf{x}) \in L^2(\overline{\Omega})$ , we have the heat distribution at time  $t$  formally as

$$u(\mathbf{x}, t) = e^{t\Delta} u_0 = \sum_{j=1}^{\infty} e^{-t\lambda_j} \langle u_0, \varphi_j \rangle \varphi_j(\mathbf{x}),$$

which is based on the expansion of the Green's function for the heat equation  $p_t(\mathbf{x}, \mathbf{y})$  via the Laplacian eigenfunctions as follows:

$$p_t(\mathbf{x}, \mathbf{y}) = \sum_{j=1}^{\infty} e^{-\lambda_j t} \varphi_j(\mathbf{x}) \overline{\varphi_j(\mathbf{y})} \quad (t, \mathbf{x}, \mathbf{y}) \in (0, \infty) \times \overline{\Omega} \times \overline{\Omega}.$$

# Solving the Heat Equation on a Complicated Domain

- Due to the discretization of the problem, we can write  $e^{t\Delta}$  in the matrix-vector notation as

$$\Phi e^{-t\Lambda} \Phi^T = \Phi \operatorname{diag} \left( e^{-t\lambda_1}, \dots, e^{-t\lambda_N} \right) \Phi^T = \sum_{j=1}^N e^{-\lambda_j t} \varphi_j \varphi_j^T,$$

where  $\Phi = (\varphi_1, \dots, \varphi_N)$  is the Laplacian eigenbasis matrix of size  $N \times N$ , and  $\Lambda$  is the diagonal matrix consisting of the eigenvalues of the Laplacian, which are the inverse of the eigenvalues of the kernel matrix, i.e.,  $\Lambda_{k,k} = \lambda_k = 1/\mu_k$ .

- Given an initial heat distribution over the domain,  $\mathbf{u}_0 \in \mathbb{R}^N$ , we can compute the heat distribution at time  $t$  as

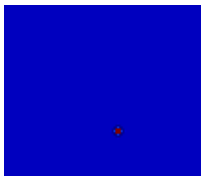
$$\mathbf{u}(t) = \Phi e^{-t\Lambda} \Phi^T \mathbf{u}_0.$$

# Solving the Heat Equation on a Complicated Domain ...

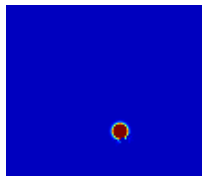
t=0



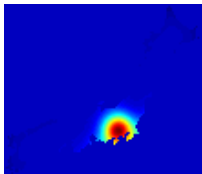
t=1



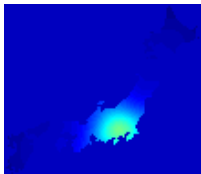
t=10



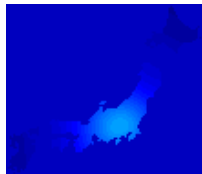
t=100



t=250



t=500



# Solving the Heat Equation on a Complicated Domain ...

- It is well known that the eigenvalues of the Laplacian with the Dirichlet (or the Neumann/Robin) boundary condition are positive (or non-negative).
- At this point, precisely specifying the boundary values is difficult because our formulation satisfies neither the Dirichlet nor the Neumann nor the Robin conditions.
- Our empirical observation so far has led to the following conjecture:

## Conjecture (NS 2007)

*The eigenvalues of the Laplacian satisfying our boundary condition and defined over a bounded domain  $\Omega \in \mathbb{R}^d$  are all positive possibly with a finite number of negative ones.*

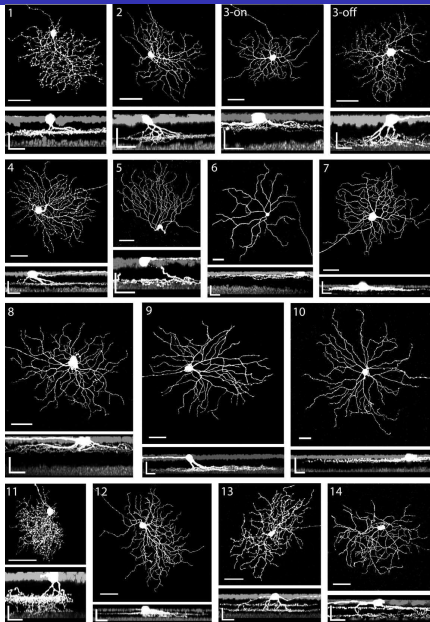
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# Clustering Mouse Retinal Ganglion Cells

- Objective: To understand how the structural/geometric properties of mouse retinal ganglion cells (RGCs) relate to the cell types and their functionality
- Why mouse?  $\implies$  great possibilities for genetic manipulation
- Data: 3D images of dendrites/axons of RGCs
- State of the Art: Process each image via specialized software to extract geometric/morphological parameters (totally 14 such parameters) followed by a conventional clustering algorithm
- These parameters include: somal size; dendritic field size; total dendrite length; branch order; mean internal branch length; branch angle; mean terminal branch length, etc.  $\implies$  takes **half a day per cell with a lot of human interactions!**

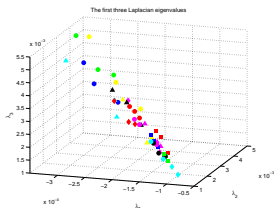
# Clustering Mouse Retinal Ganglion Cells ... 3D Data



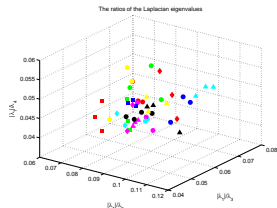
# Very Preliminary Study on Mouse Retinal Ganglion Cells

- Use 2D plane projection data instead of full 3D
- Compute the smallest  $k$  Laplacian eigenvalues using our method (i.e., the largest  $k$  eigenvalues of  $\mathcal{K}$ ) for each image
- Construct a feature vector per image
- Possible feature vectors reflecting geometric information:  
 $\mathbf{F}_1 = (\lambda_1, \dots, \lambda_k)^T$ ;  $\mathbf{F}_2 = (\mu_1, \dots, \mu_k)^T$ ;  $\mathbf{F}_3 = (\lambda_1/\lambda_2, \dots, \lambda_1/\lambda_k)^T$ ;  
 $\mathbf{F}_4 = (\mu_1/\mu_2, \dots, \mu_1/\mu_k)^T$ .
- Do visualization and clustering

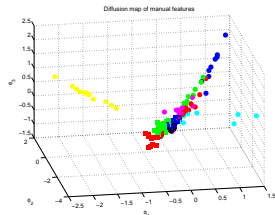
# Very Preliminary Study on Mouse RGCs ...



(a)  $F_1$

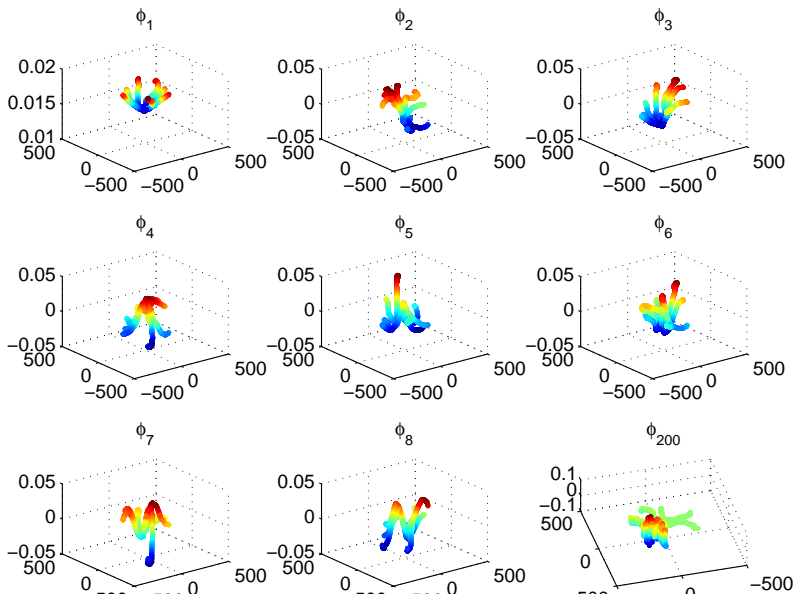


(b)  $F_3$



(c) *Manual*

# Laplacian Eigenfunctions on a Mouse RGC



# Challenges of Mouse Retinal Ganglion Cells

- Their shapes are very complicated.
- Interpretation of our eigenvalues are not yet fully understood compared to the usual Dirichlet-Laplacian case that have been well studied: the Payne-Pólya-Weinberger inequalities; the Faber-Krahn inequalities; the Ashbaugh-Benguria results, etc. For  $\Omega \in \mathbb{R}^d$ ,

$$\lambda_1^{(D)}(\Omega) \geq \left( \frac{|\mathcal{B}_1^d|}{|\Omega|} \right)^2 \lambda_1^{(D)}(\mathcal{B}_1^d), \quad \frac{\lambda_{k+1}^{(D)}(\Omega)}{\lambda_k^{(D)}(\Omega)} \leq \frac{\lambda_2^{(D)}(\mathcal{B}_1^d)}{\lambda_1^{(D)}(\mathcal{B}_1^d)}, \quad k = 1, 2, 3.$$

Note the related work on “Shape DNA” by Reuter et al. (2005), and classification of tree leaves by Khabou et al. (2007).

- Perhaps original 3D data should be used instead of projected 2D data.
- Reduce computational burden  $\implies$  need to develop fast algorithms.
- Heat propagation on the dendrites may give us interesting and useful information; after all the dendrites are network to disseminate information via chemical **reaction-diffusion** mechanism.
- Construct actual graphs based on the connectivity and analyze them directly via spectral graph theory and diffusion maps.

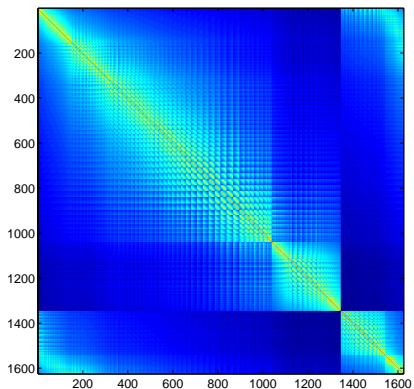
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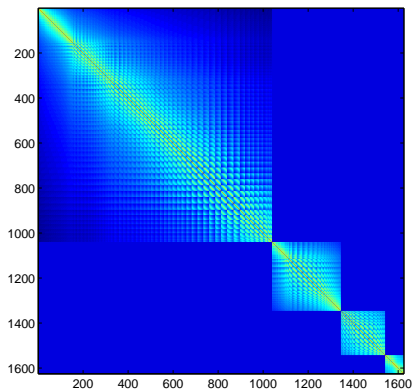
# A Possible Fast Algorithm for Computing $\varphi_j$ 's

- 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  $K\varphi$  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 Martinsson-Rokhlin-Tygert.)
- 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).

# Splitting into Subproblems for Faster Computation

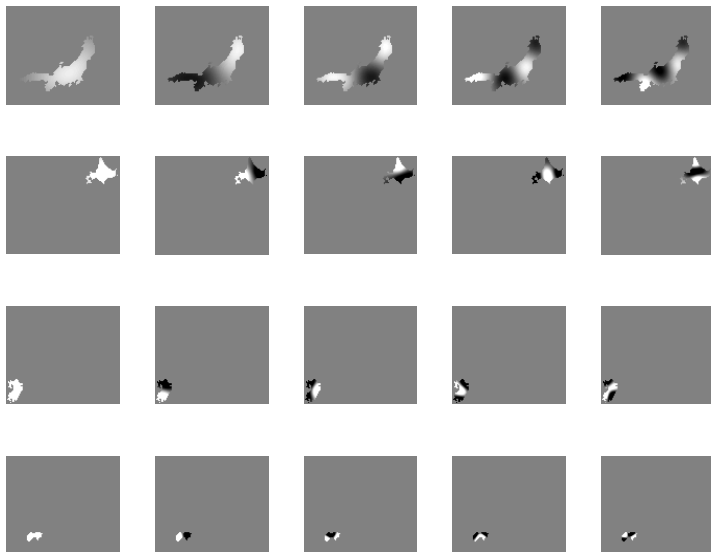


(a) Whole islands



(b) Separated islands

# Eigenfunctions for Separated Islands



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# Conclusions

- Allow **object-oriented** image analysis & synthesis
- Can get fast-decaying expansion coefficients
- Can **decouple** geometry/domain information and statistics of data
- Can extract **geometric information** of a domain through the eigenvalues
- $\exists$  A variety of applications: interpolation, extrapolation, local feature computation, ...
- **Fast algorithms** are the key for higher dimensions/large domains
- Connection to lots of interesting mathematics: spectral geometry, spectral graph theory, isoperimetric inequalities, Toeplitz operators, PDEs, potential theory, almost-periodic functions, ...
- Many things to be done:
  - Synthesize the Dirichlet-Laplacian eigenvalues/eigenfunctions from our eigenvalues/eigenfunctions
  - How about higher order, i.e., polyharmonic ?
  - Features derived from heat kernels ?
  - Improve our fast algorithm

- The following articles are available at <http://www.math.ucdavis.edu/~saito/publications/>:
- N. Saito: “Geometric harmonics as a statistical image processing tool for images defined on irregularly-shaped domains,” in *Proc. IEEE Workshop on Statistical Signal Processing*, Bordeaux, France, Jul. 2005.
- N. Saito: “Data analysis and representation using eigenfunctions of Laplacian on a general domain,” Submitted to *Applied & Computational Harmonic Analysis*, Mar. 2007.

**Thank you very much for your attention!**