Laplacian Eigenfunctions: Fast Computation via Commuting Integral Operators and Applications to Image Analysis

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Outline

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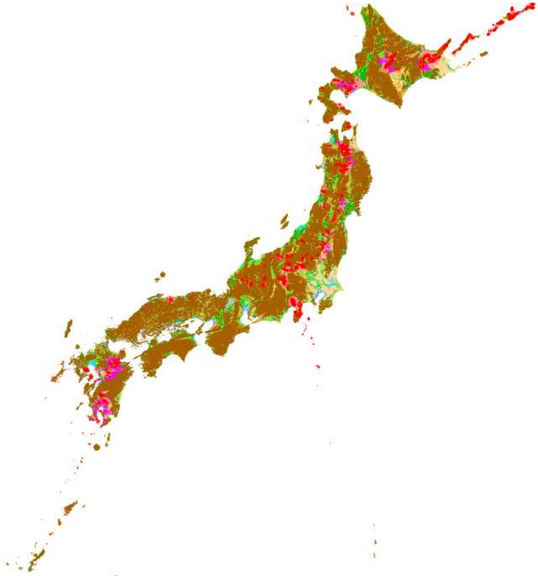
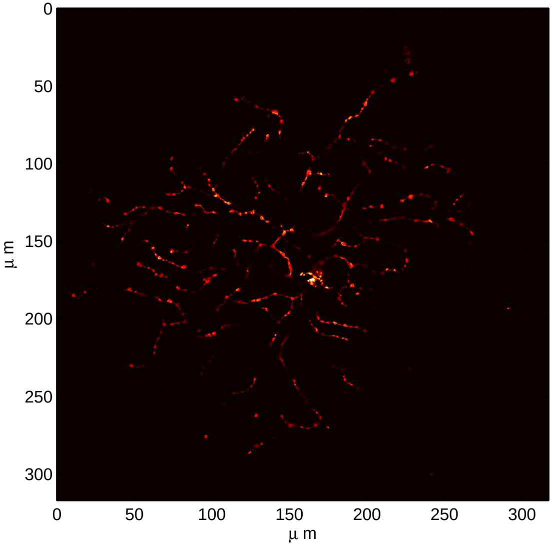
Motivations

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

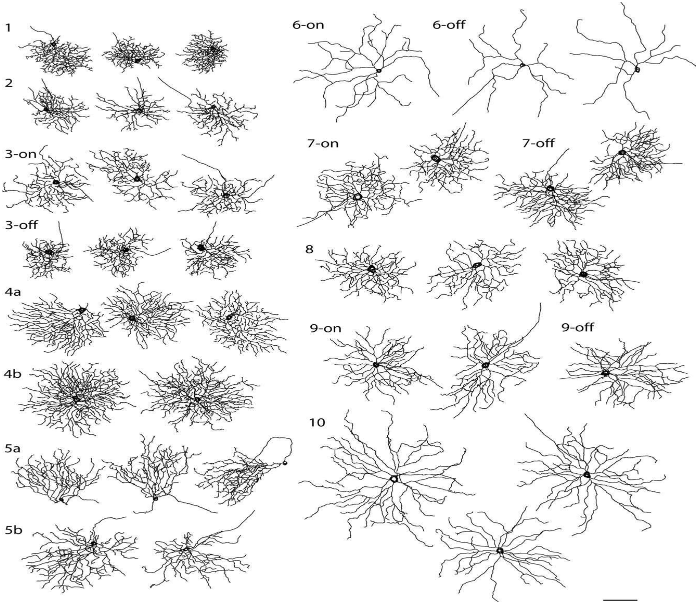
Motivations . . . Data Analysis on a Complicated Domain



Motivations . . . Clustering Complicated Objects



Motivations . . . Clustering Complicated Objects . . .



Outline

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 $L^2(\Omega)$.

Eigenfunctions of Laplacian . . . Difficulties

- The key difficulty is to compute such eigenfunctions; directly solving the Helmholtz equation (or eigenvalue problem) on a general domain is tough.
- Unfortunately, computing the Green's function for a general Ω satisfying the usual boundary condition (i.e., Dirichlet, Neumann) is also very difficult.

Outline

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

Integral Operators Commuting with Laplacian ...

- 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.

Integral Operators Commuting with Laplacian ...

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

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

Theorem (NS 2005)

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

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

for all $\mathbf{x} \in \Gamma$, where φ 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 $L^2(\Omega)$.

Outline

Outline

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 $\Longrightarrow$ 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 $\tanh \frac{\sqrt{-\lambda_0}}{2} = \frac{2}{\sqrt{-\lambda_0}}$,

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

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

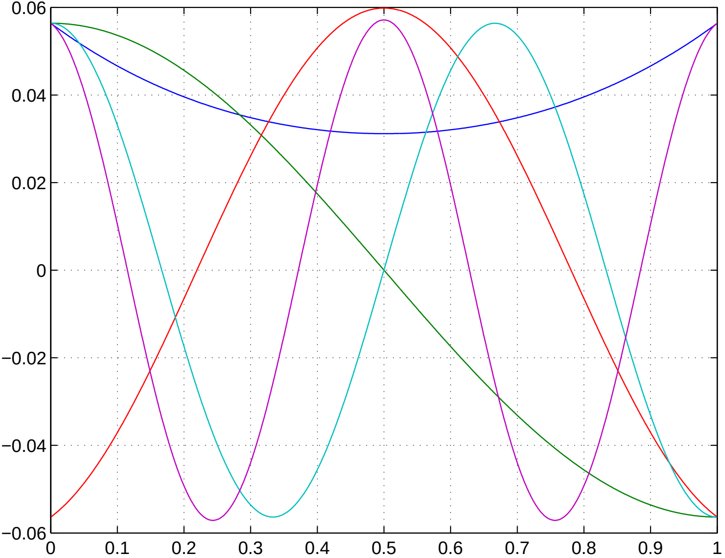
$$\varphi_{2m-1}(x) = \sqrt{2} \cos(2m-1)\pi x;$$

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

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

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

First 5 Basis Functions



Outline

2D Example

- Consider the unit disk Ω. 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:

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

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

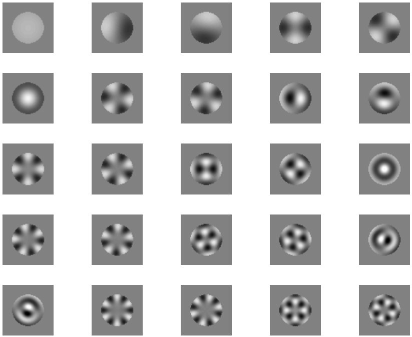
$$\mathcal{H}f(\theta) \triangleq \frac{1}{2\pi}\,\mathrm{pv}\int_{-\pi}^{\pi} f(\eta)\cot\left(\frac{\theta-\eta}{2}\right)\,\mathrm{d}\eta \quad \theta\in[-\pi,\pi].$$

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

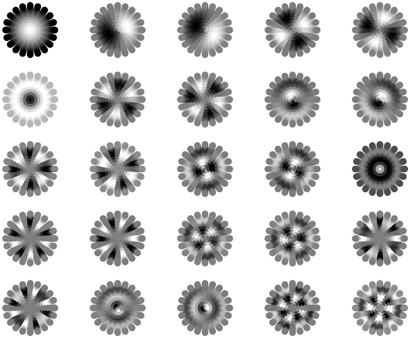
$$\varphi_{m,n}(r,\theta) = \begin{cases} J_m(\beta_{m-1,n}\,r)\binom{\cos}{\sin}(m\theta) & \text{if } m = 1,2,\ldots,\ n = 1,2,\ldots, \\ J_0(\beta_{0,n}\,r) & \text{if } m = 0,\ n = 1,2,\ldots, \end{cases}$$

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

First 25 Basis Functions



(a) Our Basis

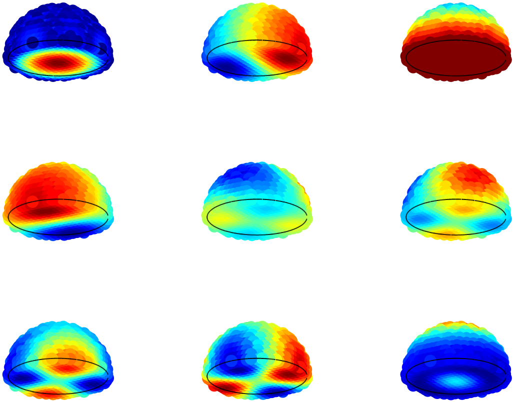


(b) Dirichlet-Laplace

Outline

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:



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 $\{\mathbf{x}_i\}_{i=1}^{N}$.
- 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.

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

- Let $K_{i,j} \triangleq w_j K(\mathbf{x}_i, \mathbf{x}_j)$, $\varphi_i \triangleq \varphi(\mathbf{x}_i)$, and $\boldsymbol{\varphi} \triangleq (\varphi_1, \ldots, \varphi_N)^T \in \mathbb{R}^N$. 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

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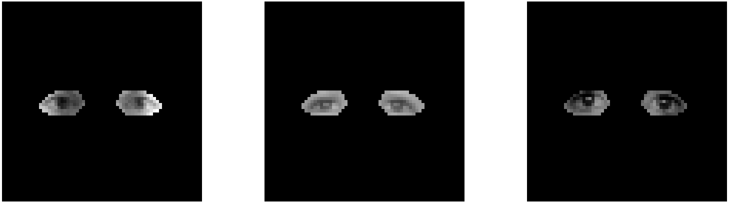
Comparison with PCA

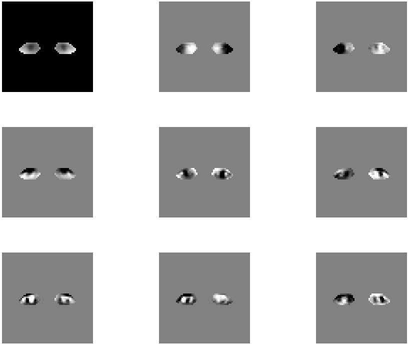
- Consider a stochastic process living on a domain Ω.
- PCA/Karhunen-Loève Transform is often used.
- PCA/KLT incorporate geometric information of the measurement (or pixel) location through the data correlation, i.e., implicitly.
- Our Laplacian eigenfunctions use explicit geometric information through 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

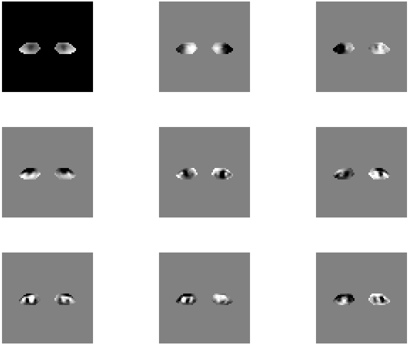


Comparison with PCA: Basis Vectors



(a) KLB/PCA 1:9

Comparison with PCA: Basis Vectors



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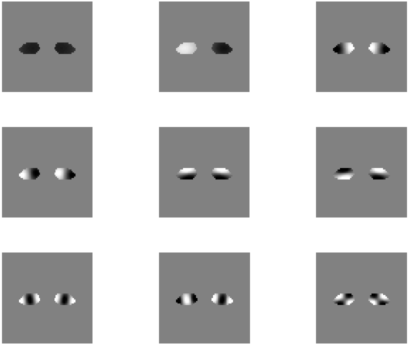
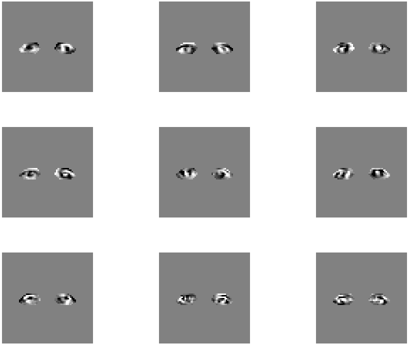
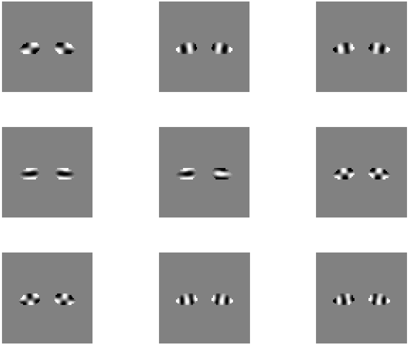


(b) Laplacian Eigenfunctions 1:9

Comparison with PCA: Basis Vectors . . .

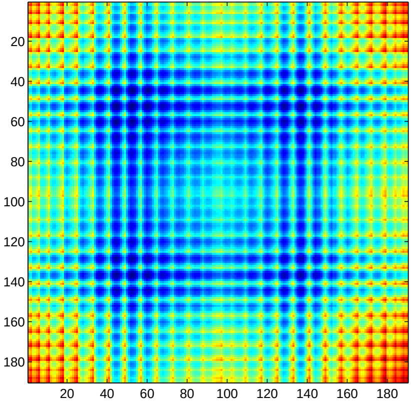


(a) KLB/PCA 10:18

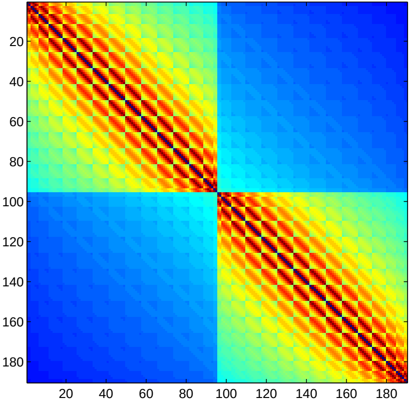


(b) Laplacian Eigenfunctions 10:18

Comparison with PCA: Kernel Matrix

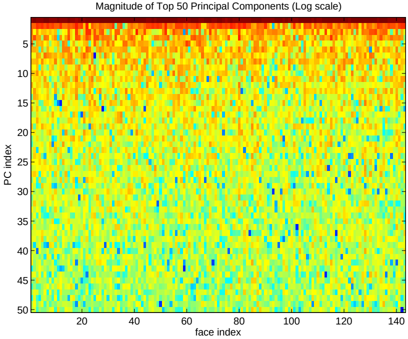


(a) Covariance

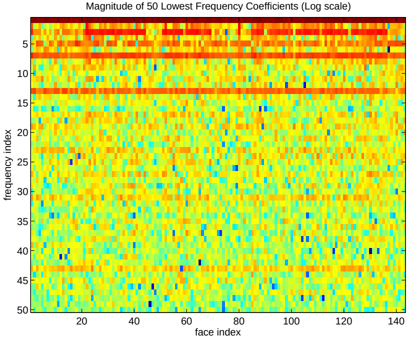


(b) Harmonic kernel

Comparison with PCA: Energy Distribution over Coordinates

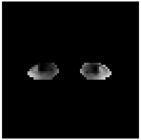


(a) KLB/PCA

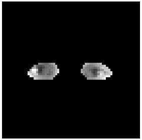


(b) Laplacian Eigenfunctions

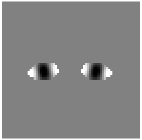
Comparison with PCA: Basis Vector #7 . . .



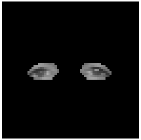
c_7:large



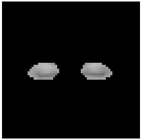
c_7:large



φ_7

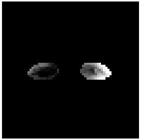


c_7:small

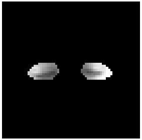


c_7:small

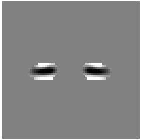
Comparison with PCA: Basis Vector #13 ...



c_{13}:large

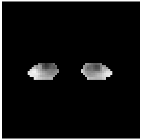


c_{13}:large



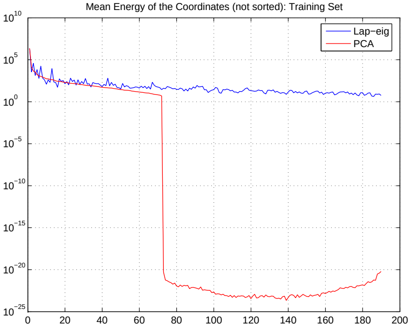
φ_{13}

c_{13}:small



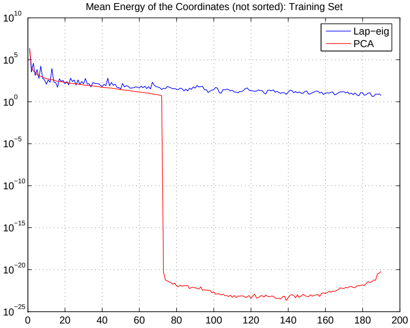
c_{13}:small

Comparison with PCA: Coefficient Decay

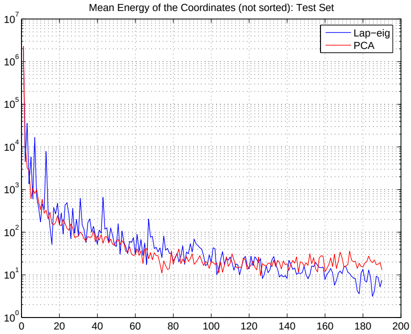


(a) Training set

Comparison with PCA: Coefficient Decay



(a) Training set



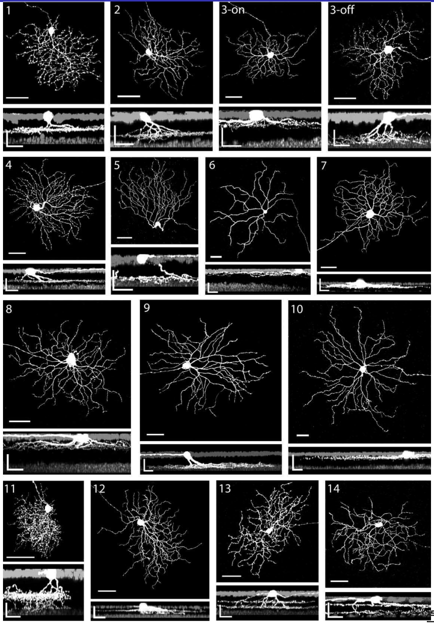
(b) Test set

Outline

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? $\Longrightarrow$ 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; dendric field size; total dendrite length; branch order; mean internal branch length; branch angle; mean terminal branch length, etc. $\Longrightarrow$ takes half a day per cell with a lot of human interactions!

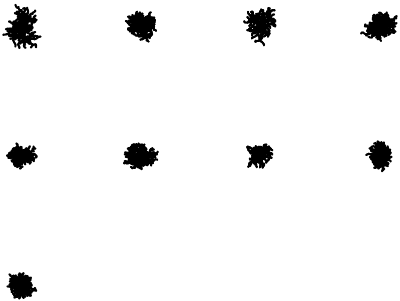
Clustering Mouse Retinal Ganglion Cells . . . 3D Data



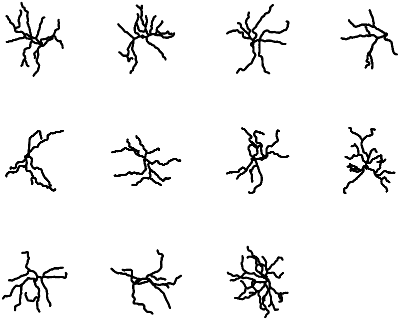
Preliminary Study on Mouse Retinal Ganglion Cells

- 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: $\mathbf{F}_1 = (\lambda_1, \ldots, \lambda_k)^T$; $\mathbf{F}_2 = (\mu_1, \ldots, \mu_k)^T$; $\mathbf{F}_3 = (\lambda_1/\lambda_2, \ldots, \lambda_1/\lambda_k)^T$; $\mathbf{F}_4 = (\mu_1/\mu_2, \ldots, \mu_1/\mu_k)^T$.
- Do visualization and clustering

Preliminary Study on Mouse RGCs . . .

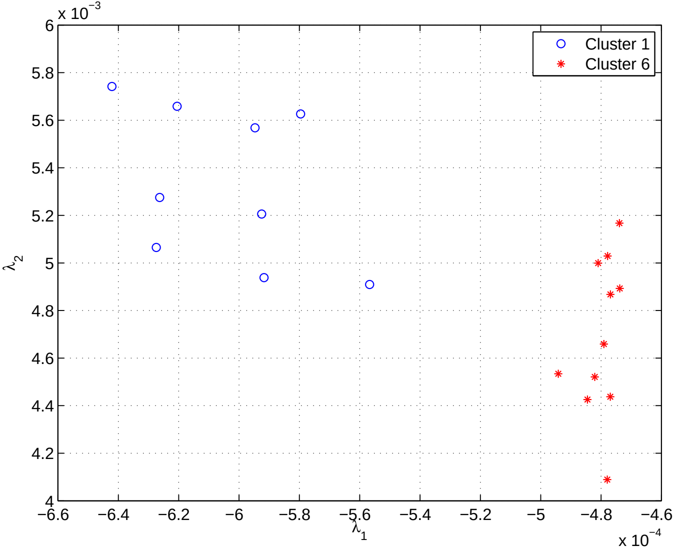


(a) Cluster 1

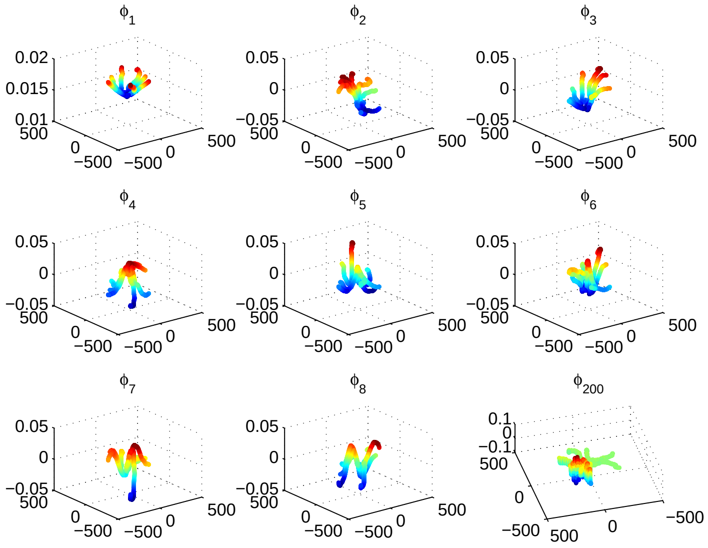


(b) Cluster 6

Crossplot of the First Two Laplacian Eigenvalues



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 $\Omega \in \mathbb{R}^d$,

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

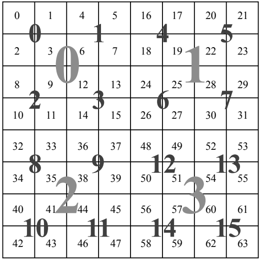
  Note the related work on "Shape DNA" by Reuter et al. (2005), and classification of tree leaves by Khabou et al. (2007).
- Perhaps original 3D data should be used instead of projected 2D data.
- Reduce computational burden $\Longrightarrow$ need to develop fast algorithms.
- Heat propagation on the dendrites 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.

Outline

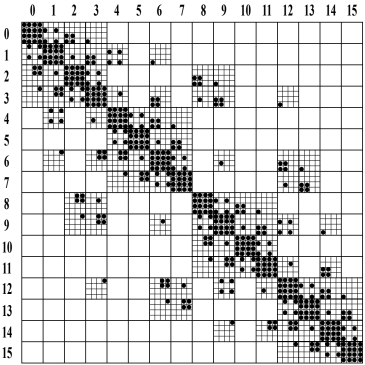
A Possible Fast Algorithm for Computing φ_j's

- 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 $K\varphi$ 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).

Tree-Structured Matrix via FMM

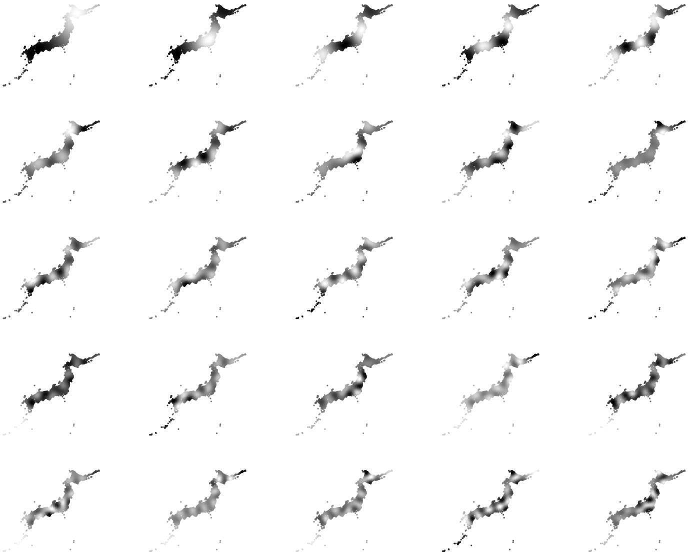


(a) Hierarchical indexing scheme

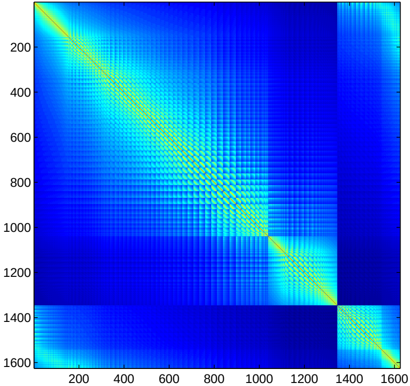


(b) Tree-Structured Matrix

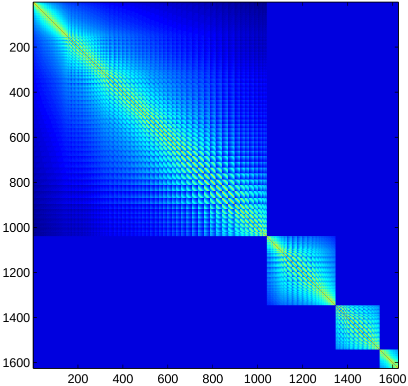
First 25 Basis Functions via the FMM-based algorithm



Splitting into Subproblems for Faster Computation

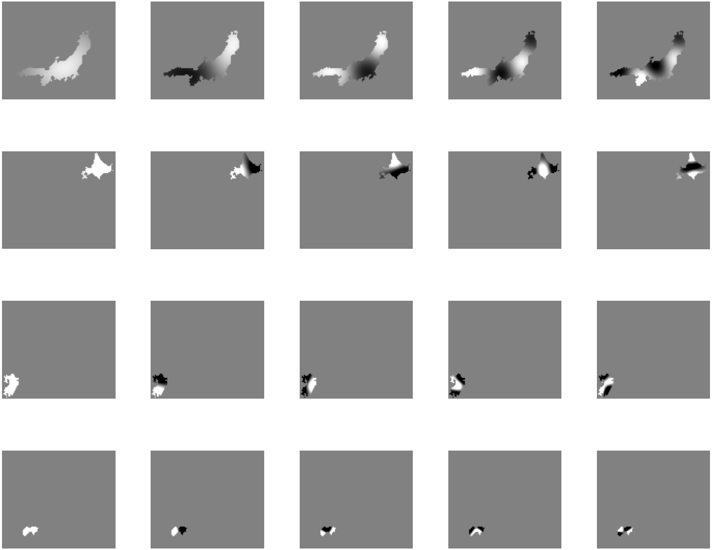


(a) Whole islands



(b) Separated islands

Eigenfunctions for Separated Islands



Outline

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, solving heat equations on complicated domains . . .
- 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

References

- 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!