Discrete Integral Operators and Distance Matrices for Graph Signal Processing

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Naoki Saito

UC Davis TETRAPODS Institute of Data Science
Department of Mathematics, University of California, Davis

Outline

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Acknowledgment

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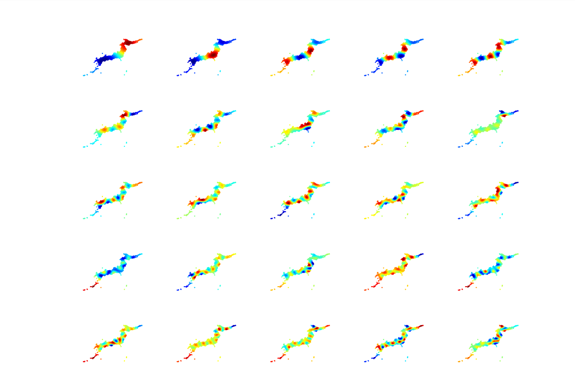
- And my collaborator on this project:

Eugene Shvarts (UCD → Teleport)

Outline

Motivations

Since 2005 or so, I have been studying the *integral operators that commute with the Laplace operators* on various domains ranging from simple Euclidean domains (e.g., the 1D unit interval or the 2D unit circle) to very complicated 2D domains (e.g., the Japanese archipelago) to graphs.

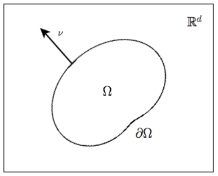


Motivations: Why commuting integral operators?

- Easier to implement than differential operators that require specification of precise *boundary conditions*
- Utilize *global* information (e.g., shortest distances between points) instead of *local* information (e.g., communication with immediate neighbors in differential operators)
- Easier to handle *directed graphs* than differential operators
- *Numerically more stable* in eigenvalue solvers than discretized differential operators
- Lead to dense kernel matrices yet $\exists$ an efficient computational algorithm for eigenvalue solvers, i.e., the *Fast Multipole Method* (FMM)

Motivations: Why Laplacian Eigenfunctions on $\Omega \in \mathbb{R}^d$?

- 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.



Enter Laplacian Eigenfunctions!

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

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

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

Laplacian Eigenfunctions: Some Facts

- 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!*

Laplacian Eigenfunctions: Difficulties

- 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 $L^2(\Omega)$.
- The key difficulty is to compute such eigenfunctions; directly solving the *Helmholtz equation* (or eigenvalue problem) on a general domain is tough.
- Unfortunately, computing the Green's function for a general Ω satisfying the usual boundary condition (i.e., Dirichlet, Neumann, Robin) is also very difficult.

Outline

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

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.

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 2008)

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

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

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

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.

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

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

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

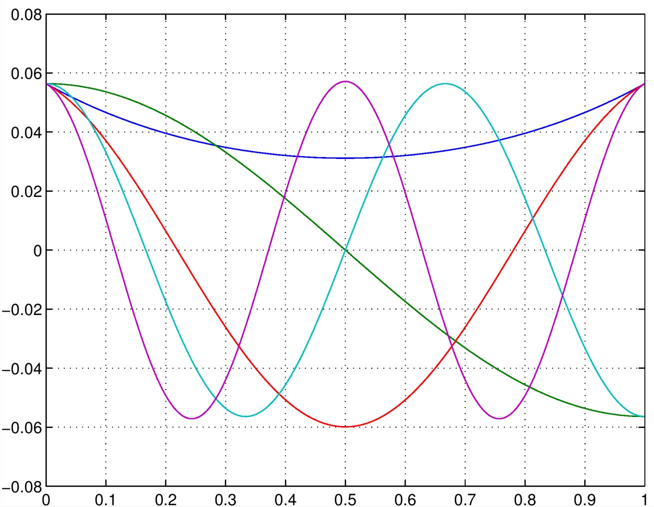
$$\varphi_{2m-1}(x) = \sqrt{2}\cos(2m-1)\pi x;$$

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

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

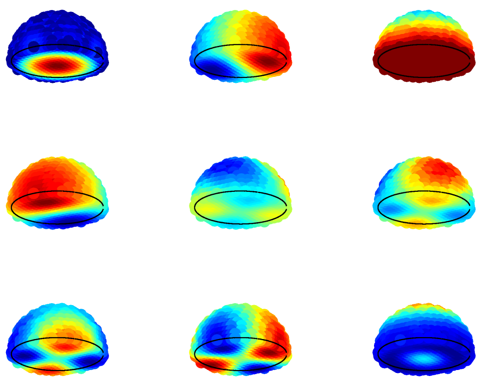
where A_k, $k = 0, 1, \ldots$ are normalization constants.

First 5 Basis Functions



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

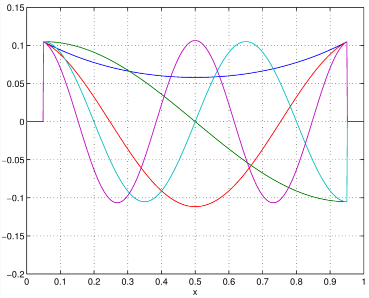
Incorporating the DC Vector

- 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 $\mathrm{span}\{\boldsymbol{\chi}_\Omega\}$ in the column space of the kernel matrix K:

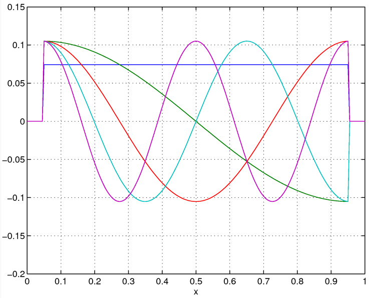
$$\widetilde{K} = \left(I - \boldsymbol{\chi}_\Omega \boldsymbol{\chi}_\Omega^\mathsf{T}\right) K =: PK.$$

- Then, $\boldsymbol{\chi}_\Omega$ together with the eigenvectors of $\widetilde{K}$ corresponding to the largest $n-1$ eigenvalues form the desired orthonormal basis.

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?*

Relationship with the Neumann-Laplacian for $\Omega \in \mathbb{R}^1$

- It turned out that there is more to the DC vector business!
- The eigenfunctions of the *Neumann-Laplacian* automatically includes the DC vector of a domain.
- Hence, it is natural to investigate the relationship between our integral operator $\mathscr{K}$ and the Neumann-Laplacian $\mathscr{L}_N$.
- Then, consider $\mathscr{P}\mathscr{K}\mathscr{P}$, with $\mathscr{P}$ the orthogonal projection onto the orthogonal complement of the DC component $\mathrm{span}\{\boldsymbol{\chi}_\Omega\}$.

Theorem

Let $\Omega = (0,1) \in \mathbb{R}$. Then, the kernel of the integral operator $\mathscr{P}\mathscr{K}\mathscr{P}$ is precisely the Neumann Green's function G_N. In particular, $(\mathscr{P}\mathscr{K}\mathscr{P})\,\mathscr{L}_N = \mathscr{L}_N\,(\mathscr{P}\mathscr{K}\mathscr{P})$.

Neumann conditions tied intimately to projections:

- $\partial_\nu f\big|_{\partial\Omega} = 0 \implies \mathscr{P}\mathscr{L}_N f = \mathscr{L}_N f$
- $\int_\Omega f = 0 \iff \mathscr{P} f = f$

Relationship with the graph Laplacian

- Let's consider the discrete case, i.e., the *midpoint* discretization of $(0,1)$, which leads to a *path graph* P_n consisting of n nodes.
- Let L, K, P denote the graph Laplacian, the discretized integral operator, and the orthogonal projector killing the DC component, corresponding to $\mathscr{L}$, $\mathscr{K}$, $\mathscr{P}$ in the continuum, respectively.

Theorem

$PKP = L^{\dagger}$. *In particular,* $(PKP)L = L(PKP)$.

- Consequently, the eigenvectors of PKP are *exactly the DCT Type II basis vectors* used for the JPEG standard.
- Knowledge of $K \iff$ *distance matrix* Δ of P_n. In fact, for P_n, $K = -\Delta/2$.

Higher dimensions: Neumann BC's; Generalized DCT

- $\mathscr{PKP}$ commutes with a *subspace* of the domain of the Neumann-Laplacian:

Theorem

Let Ω be a sufficiently smooth bounded domain in $\mathbb{R}^d$, $d \geq 2$, and let f satisfy both $\partial_\nu f\big|_{\partial\Omega} \equiv 0$, and $\int_\Omega f = 0$. Then $(\mathscr{PKP})\mathscr{L}_N f = \mathscr{L}_N(\mathscr{PKP}) f = f$ if and only if $f\big|_{\partial\Omega} \equiv \mathrm{const}$.

- For *some* discretized domains, we can say the following:

Theorem

Let G be either a tree or a lattice graph $P_{n_1} \otimes \cdots \otimes P_{n_d}$ in $\mathbb{R}^d$. Let L, Δ be the graph Laplacian, the distance matrix of G. Then, $(P\Delta P)L = L(P\Delta P)$. Hence, in the lattice case, the eigenvectors of $P\Delta P$ are the tensor-product DCT-II vectors.

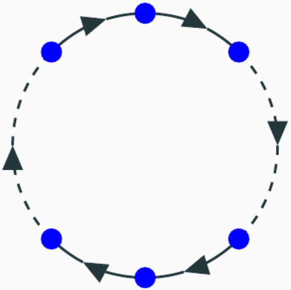
- *What is the right kernel for the integral operator for general graphs?*

Outline

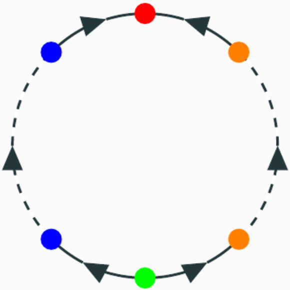
Handling Directed Graphs with Integral Operators

- If G is a directed graph (digraph), then its graph Laplacian $L(G) := D(G) - W(G)$ is nonsymmetric $\Longrightarrow$ not necessarily diagonalizable; eigenvalues may be in $\mathbb{C}$; $\exists$ many different definitions of $L(G)$ ...
- Our viewpoint: the connectivity between any two vertices in a digraph are not a local concept; rather it is a *global* concept. Think about one-way streets in your town!
- Hence, it is quite natural to use the *distance matrix* of G, $\Delta(G) := (d(i,j))_{i,j=1:n}$ where $d(i,j)$ is *the shortest/geodesic distance* between vertices i, j.
- Note that if edge weights of G reflect the *affinity* instead of the distance, then $d(i,j)$ should be the sum of the edge weights along the greatest affinity path between i, j.
- Our previous investigation suggests the *SVD* of $K(G)$ and $PK(G)P$. Note that in 3D, $K(G) = \frac{1}{4\pi}(1/d(i,j))_{i,j}$.

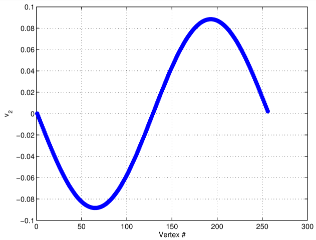
Detecting the directional difference!



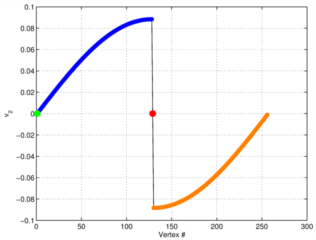
(a) A directed circle



(b) *Not* strongly connected version

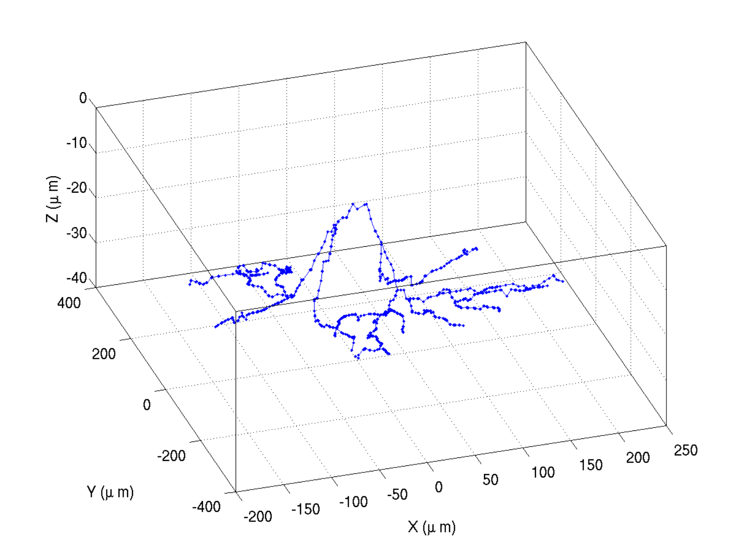


(c) $\boldsymbol{v}_2$



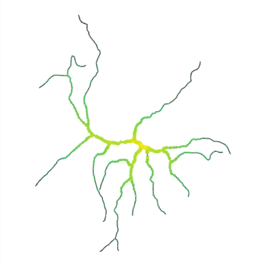
(d) $\boldsymbol{v}_2$

Example: A Neuronal Dendritic Tree

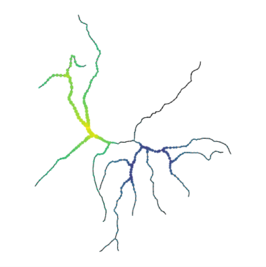


Mouse's retinal ganglion cell as a tree ($n = 1154$)

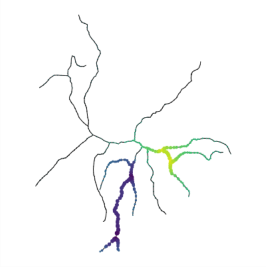
Right Singular Vectors of K vs PKP for *undirected* case



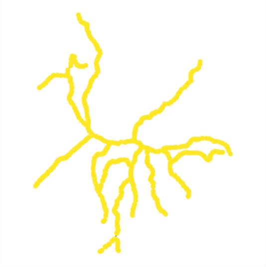
(a) $\boldsymbol{v}_1$



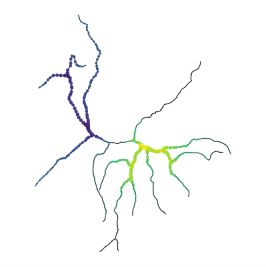
(b) $\boldsymbol{v}_2$



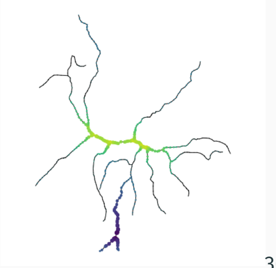
(c) $\boldsymbol{v}_3$



(d) $\tilde{\boldsymbol{v}}_{1154}$

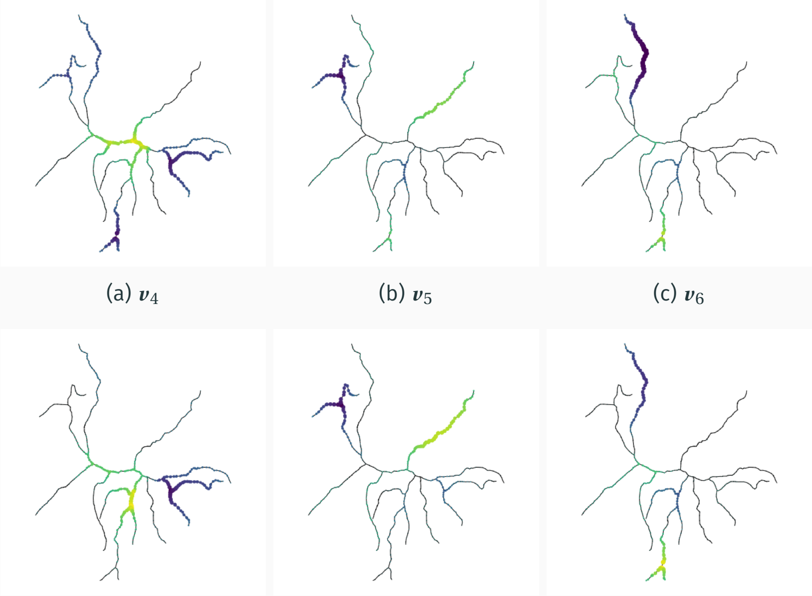


(e) $\tilde{\boldsymbol{v}}_1$



(f) $\tilde{\boldsymbol{v}}_2$

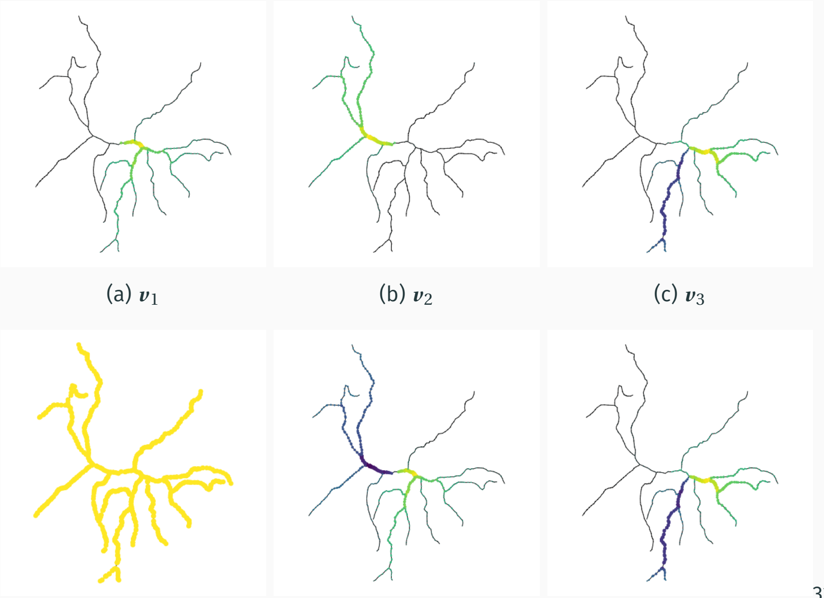
Right Singular Vectors of K vs PKP for *undirected* case ...



(a) $\boldsymbol{v}_4$ (b) $\boldsymbol{v}_5$ (c) $\boldsymbol{v}_6$

(d) $\tilde{\boldsymbol{v}}_3$ (e) $\tilde{\boldsymbol{v}}_4$ (f) $\tilde{\boldsymbol{v}}_5$

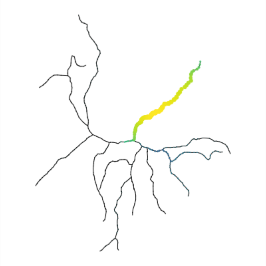
Right Singular Vectors of K vs PKP for *directed* case



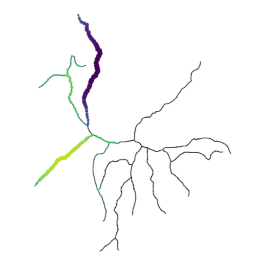
(a) $\boldsymbol{v}_1$ (b) $\boldsymbol{v}_2$ (c) $\boldsymbol{v}_3$

(d) $\tilde{\boldsymbol{v}}_{1154}$ (e) $\tilde{\boldsymbol{v}}_1$ (f) $\tilde{\boldsymbol{v}}_2$

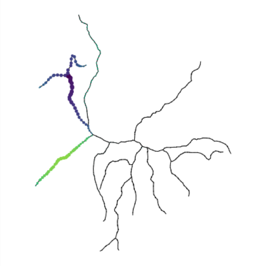
Right Singular Vectors of K vs PKP for *directed* case ...



(a) $\boldsymbol{v}_4$

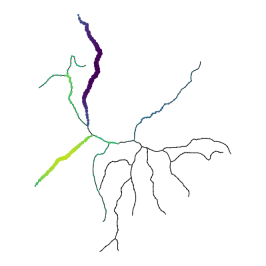


(b) $\boldsymbol{v}_5$

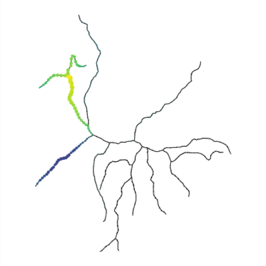


(c) $\boldsymbol{v}_6$

(d) $\tilde{\boldsymbol{v}}_3$

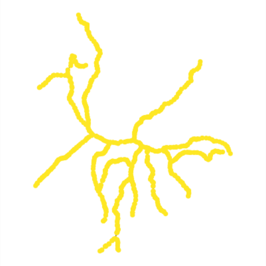


(e) $\tilde{\boldsymbol{v}}_4$

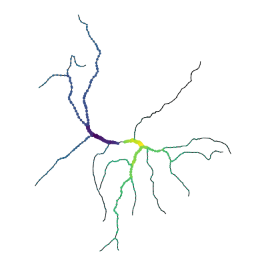


(f) $\tilde{\boldsymbol{v}}_5$

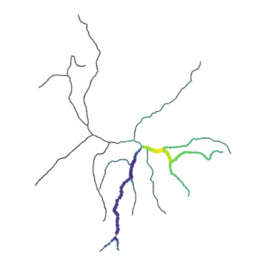
Right Singular Vectors PKP for the *different directed* cases



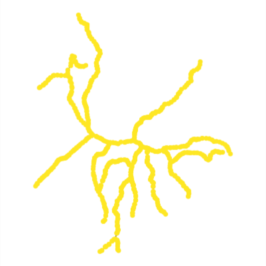
(a) $\tilde{\boldsymbol{v}}_{1154}$



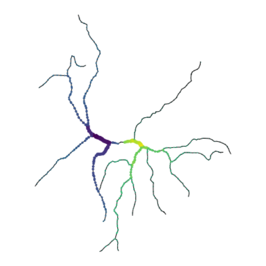
(b) $\tilde{\boldsymbol{v}}_{1}$



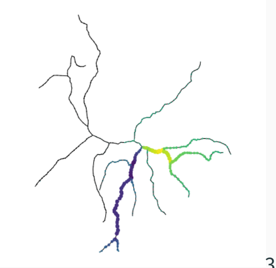
(c) $\tilde{\boldsymbol{v}}_{2}$



(d) $\tilde{\tilde{\boldsymbol{v}}}_{1154}$

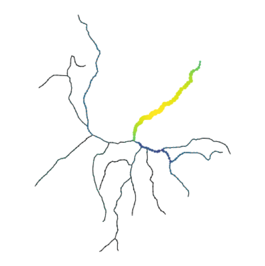


(e) $\tilde{\tilde{\boldsymbol{v}}}_{1}$

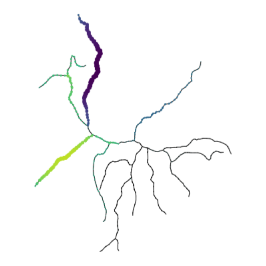


(f) $\tilde{\tilde{\boldsymbol{v}}}_{2}$

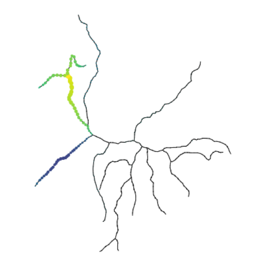
Right Singular Vectors PKP for the *different directed* cases ...



(a) $\tilde{\boldsymbol{v}}_3$

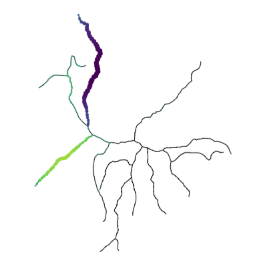


(b) $\tilde{\boldsymbol{v}}_4$

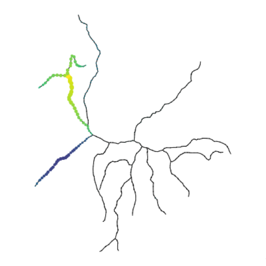


(c) $\tilde{\boldsymbol{v}}_5$

(d) $\tilde{\tilde{\boldsymbol{v}}}_3$



(e) $\tilde{\tilde{\boldsymbol{v}}}_4$



(f) $\tilde{\tilde{\boldsymbol{v}}}_5$

Outline

Summary

Our approach using the commuting integral operators

- Allows data analysis analysis & synthesis on quite singular domains including graphs
- is based on the *distance matrix* of the sample points on the domain, closely related to the *Green's function*
- Can get *fast-decaying expansion coefficients* (less Gibbs effect)
- Can handle data analysis/synthesis on *directed graphs*
- Can incorporate the *DC vector* of a domain if a user wishes, which leads to the *generalized discrete cosine transform*

Furthermore, our approach

- 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*
- Can use the *Fast Multipole Method* to speed up the computation, which is the key for higher dimensions/large domains
- Has a connection to lots of interesting mathematics: spectral geometry, spectral graph theory, isoperimetric inequalities, Toeplitz operators, PDEs, potential theory, almost-periodic functions, ...

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Future Plan

- Investigate numerical quadratures for more accurate discrete integral operators on *irregularly-sampled domains and graphs*
- Extend our integral operator to *Hodge Laplacians* for *simplicial complexes*; see, e.g., [S-Schonsheck-Shvarts (2024)]
- Develop *wavelet packets* on a general shape domain by hierarchically grouping the eigenfunctions similar to what we did recently for graphs [Cloninger-Li-S (2021)]
- Examine further our boundary conditions for specific geometry in higher dimensions; e.g., analysis of $\mathbb{S}^2$ leads to *Clifford Analysis*
- Integral operators commuting with *polyharmonic operators* $(-\Delta)^p$, $p \geq 2$; *Helmholtz operators* $\Delta + k^2$; etc.
- Investigate the *heat kernel* in $\mathbb{R}^d$:
  $K_t(\boldsymbol{x}, \boldsymbol{y}) := \exp(t\Delta)(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{(4\pi t)^{d/2}} \mathrm{e}^{-\|\boldsymbol{x}-\boldsymbol{y}\|^2/4t}$

Outline

References

Laplacian Eigenfunction Resource Page: https://www.math.ucdavis.edu/~saito/lapeig/ contains my course note: “Laplacian Eigenfunctions: Theory, Applications, and Computations” as well as other useful information

The following articles are available at https://www.math.ucdavis.edu/~saito/publications/ :

- N. Saito: “Data analysis and representation using eigenfunctions of Laplacian on a general domain,” *Applied & Computational Harmonic Analysis*, vol. 25, no. 1, pp. 68–97, 2008.
- L. Hermi & N. Saito: “On Rayleigh-type formulas for a non-local boundary value problem associated with an integral operator commuting with the Laplacian,” *Applied & Computational Harmonic Analysis*, vol. 45, no. 1, pp. 59–83, 2018.
- A. Cloninger, H. Li, & N. Saito: “Natural graph wavelet packet dictionaries,” *Journal of Fourier Analysis & Applications*, vol. 27, article #41, 2021.
- L. Hermi & N. Saito: “On a nonlocal integral operator commuting with the Laplacian and the Sturm-Liouville Problem I: Low rank perturbations of the operator,” arXiv:2211.07141v3 [math.SP], 2023.
- N. Saito, S. Schonsheck, & E. Shvarts: “Multiscale transforms for signals on simplicial complexes,” *Sampling Theory, Signal Processing, and Data Analysis*, vol. 22, no. 2, 2024.

Thank you very much for your attention!