Three Excursions around Laplacians

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GGAM Colloquium
April 6, 2017

Outline

Acknowledgment

- ONR Grants: N00014-00-1-0469; N00014-06-1-0615; N00014-07-1-0166; N00014-09-1-0041; N00014-09-1-0318; N00014-12-1-0177; N00014-16-1-2255
- NSF Grants: DMS-0410406; DMS-1418779
- Faisal Beg (Simon Fraser Univ., Canada)
- Leo Chalupa (George Washington Univ.)
- Tim DelSole (George Mason Univ.)
- Lotfi Hermi (Univ. Arizona)
- John Hunter (UC Davis)
- Jeff Irion (Bosch, Inc.)
- Yuji Nakatsukasa (Oxford Univ.)
- Jean François Remy (DriveScale, Inc.)
- Ernest Woei (Trendage, Inc.)
- Allen Xue (Amgen, Inc.)
- Katsu Yamatani (Meijo Univ., Japan)
- The MacTutor History of Mathematics Archive, Wikipedia, . . .

Outline

Introductory Comments

Hajime Urakawa (Emeritus Prof., Tohoku Univ.) said in 1999:

> *A long time ago, when I was a college student, I was told: "There is good mathematics around Laplacians." I engaged in mathematical research and education for a long time, but after all, I was just walking around "Laplacians," which appear in all sorts of places under different guises. When I reflect on the above proverb, however, I feel keenly that it represents an aspect of the important truth. I was ignorant at that time, but it turned out that "Laplacians" are one of the keywords to understand the vast field of modern mathematics.*

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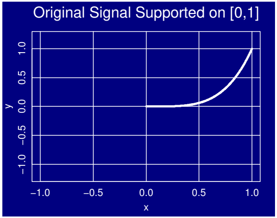
I second Prof. Urakawa's opinion, and want to add: *"There are good applications around Laplacians too."*

Outline

Motivations

I always felt frustrated to deal with data supported on an interval in 1D or a rectangle in 2D/3D using Fourier series or its discrete counterpart, DFT.



(a) Original Signal

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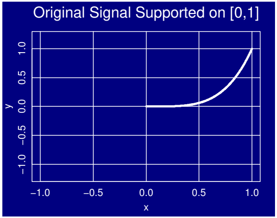

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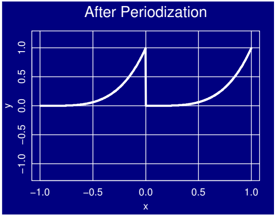

(b) Periodized Signal

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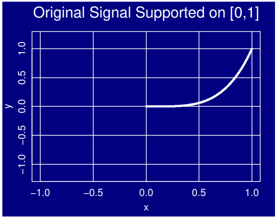

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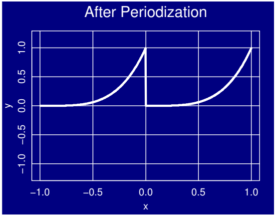
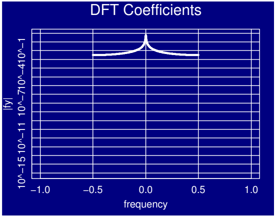


(b) Periodized Signal



(c) |DFT of (b)|

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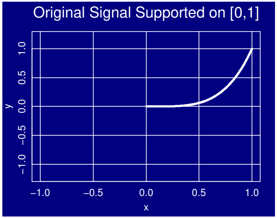

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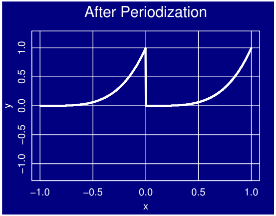
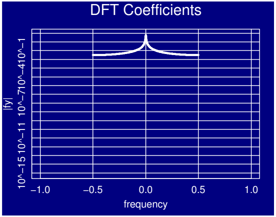


(b) Periodized Signal



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Let f_{per} be a periodized version of f with $\operatorname{supp} f = [0,1]$. Then, the expansion coefficients $\{c_k = \langle f_{\text{per}}, \mathrm{e}^{2\pi \mathrm{i} k \cdot} \rangle\}_{k \in \mathbb{Z}}$ of the Fourier series of a periodic function $f_{\text{per}}(x) \sim \sum_k c_k \mathrm{e}^{2\pi \mathrm{i} k x}$ *decay slowly*, i.e., $O(1/|k|)$ as $|k| \to \infty$ if f_{per} is *discontinuous*.

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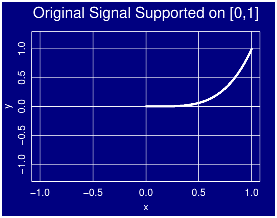

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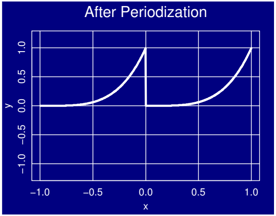
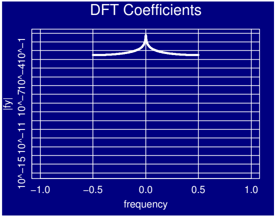


(b) Periodized Signal



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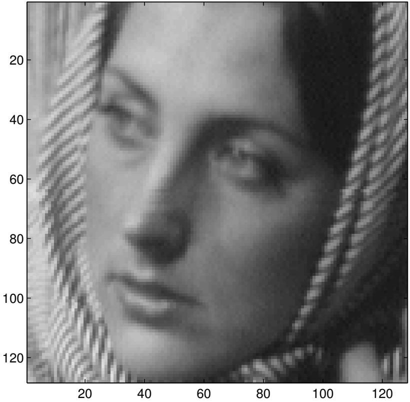
$\Longrightarrow$ This could happen even if $f \in C^\infty[0,1]$!

- It is important to have *fast decaying* or *sparse* expansion coefficients in many applications.
- For example, slowly decaying expansion coefficients relative to Discrete Cosine Transform (DCT) used in the JPEG standard degrade quality of images:



(a) Original: 8 bpp (bits/pixel)

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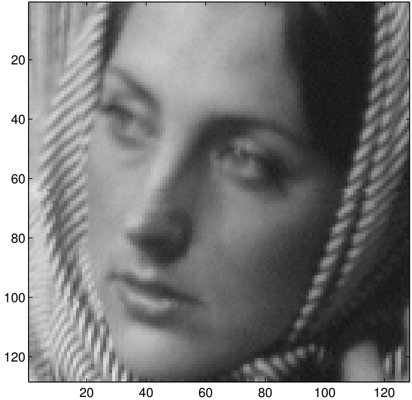

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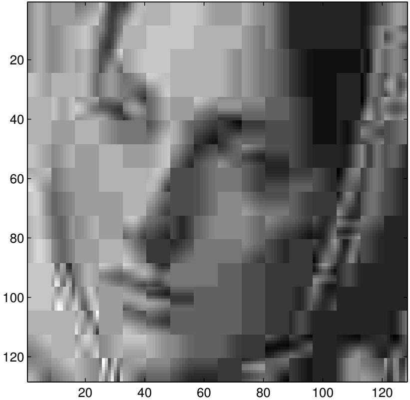

(b) JPEG: 0.162 bpp

- Wanted to develop a *local* image transform that generates faster decaying expansion coefficients than block DCT used in JPEG without using popular sliding window-based techniques
- Wanted to fully incorporate the *infrastructure* provided by the JPEG standard, e.g., the block DCT algorithm, the quantization method, the file format, etc.

Review of Fourier Cosine Series

- Let $\Omega = (0,1)^2 \subset \mathbb{R}^2$ and $f \in C^2(\overline{\Omega})$ but not periodic: the periodically extended version of f is *discontinuous* at $\partial\Omega$.
- Then the size of the complex Fourier coefficients $c_{\boldsymbol{k}}$ of f decay as $O(\|\boldsymbol{k}\|^{-1})$, where $\boldsymbol{k} = (k_1, k_2) \in \mathbb{Z}^2$.
- Instead, expanding f into the Fourier *cosine* series gives rise to the decay rate $O(\|\boldsymbol{k}\|^{-2})$ because it is equivalent to the complex Fourier series expansion of the extended version of f via *even reflection that is continuous at $\partial\Omega$*.
- This is one of the main reasons why the JPEG adopts DCT instead of Discrete Fourier Transform (DFT) or Discrete Sine Transform (DST)

- How about using *Chebyshev polynomials*? $\Longrightarrow$ Unfortunately, usual signals and images are sampled on the equispaced grid points, not on the Chebyshev nodes.

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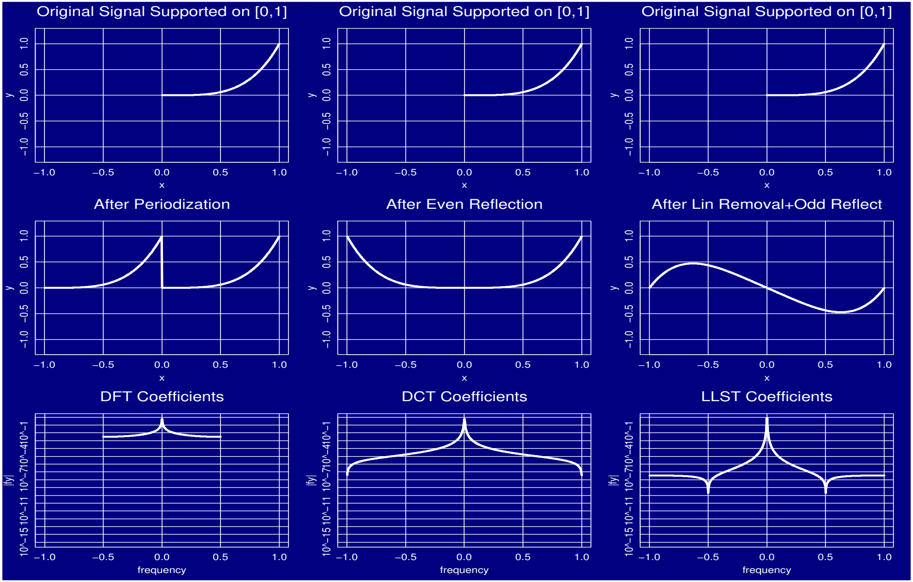
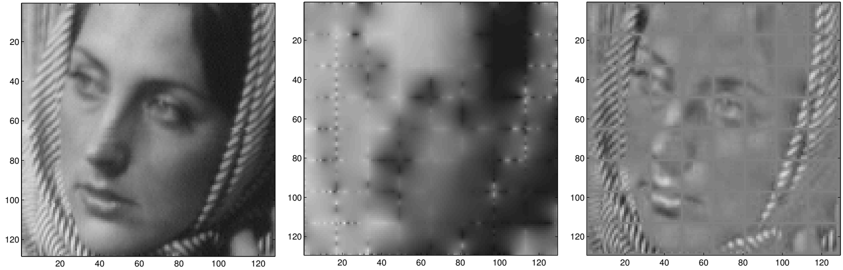
Review of Polyharmonic Local *Sine* Transform

- We now consider a decomposition $f = u + v \in C^2(\overline{\Omega})$.
- The u (or polyharmonic) component satisfies *Laplace's equation with the Dirichlet boundary condition*:

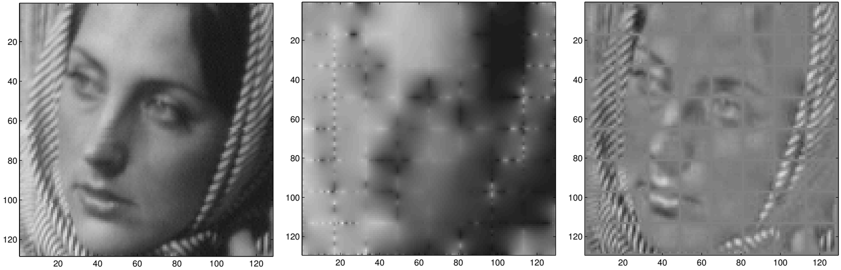
$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad \text{in } \Omega; \qquad u = f \quad \text{on } \partial\Omega.$$

- The u component is solely represented by the boundary values of f via the fast and highly accurate Dirichlet problem solver of Averbuch, Israeli, & Vozovoi (1998).
- The residual $v = f - u$ *vanishes* on $\partial\Omega \Longrightarrow$ The Fourier *sine* coefficients of v decay as $O(\|\boldsymbol{k}\|^{-3})$ because $\tilde{v}$, the *odd* extension of v to $\tilde{\Omega} := [-1,1]^2$, becomes a *periodic* $C^1(\tilde{\Omega})$ function.
- This is a multidimensional extension of the idea of Lanczos (1938).
- In higher dimensions, *harmonic functions* are easier to deal with than algebraic polynomials; See [Saito-Remy 2006] for the details.


Original Signal Supported on [0,1]
Original Signal Supported on [0,1]
Original Signal Supported on [0,1]
After Periodization
After Even Reflection
After Lin Removal+Odd Reflect
DFT Coefficients
DCT Coefficients
LLST Coefficients
x
y
frequency
|fy|
−1.0 −0.5 0.0 0.5 1.0
10^−15 10^−11 10^−7 10^−4 10^−1



(a) Original (b) $\cup_j u_j$ (c) $\cup_j v_j$



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PHLST was a nice idea and published in a good journal, but ...

Polyharmonic Local Cosine Transform

- Wanted to use DCT for fully utilizing the JPEG infrastructure
- Wanted coefficients decaying faster than $O(\|\boldsymbol{k}\|^{-3})$
- To do so, we need to solve *Poisson's equation with the Neumann boundary condition*:

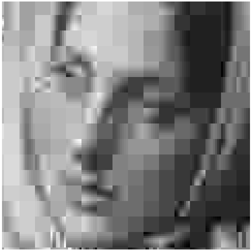
$$\Delta u = K \quad \text{in } \Omega; \qquad \partial_\nu u = \partial_\nu f \quad \text{on } \partial\Omega,$$

  where the constant source term $K := \frac{1}{|\Omega|} \int_{\partial\Omega} \partial_\nu f(\boldsymbol{x})\, \mathrm{d}\sigma(\boldsymbol{x})$ is necessary for the solvability of the Neumann problem, which forces us to use Poisson's equation instead of Laplace's equation.
- Then, the Fourier *cosine* coefficients of the residual decay as $O(\|\boldsymbol{k}\|^{-4})$ because $\tilde{v}$, the *even* extension of v to $\tilde{\Omega}$ becomes a *periodic* $C^2(\tilde{\Omega})$ function thanks to $\partial_\nu v = 0$ on $\partial\Omega$.

Computational Aspects of PHLCT

- Wanted to achieve the PHLCT representation of $f = u + v$ entirely in the DCT domain, $F = U + V$, which turned out possible because:
  1. an approximation of U can be computed using $F_{0,0}$ (= the DC component of F) and those of the surrounding blocks; and
  2. we can set $V_{0,0} = F_{0,0}$.
- Full mode PHLCT (FPHLCT) adds simple procedures in both the encoder and the decoder parts of the JPEG Baseline method.
- Partial mode PHLCT (PPHLCT) modifies only the decoder part of the JPEG Baseline method: *PPHLCT accepts the JPEG-compressed files!*
- Essentially, the JPEG tends to kill $F_{\boldsymbol{k}}$ for large $\boldsymbol{k}$, but PPHLCT replaces it by $U_{\boldsymbol{k}}$, which is reasonable because $V_{\boldsymbol{k}}$ is expected to decay quickly, i.e., $F_{\boldsymbol{k}} \approx U_{\boldsymbol{k}}$ for large $\boldsymbol{k}$.
- No time to discuss the algorithmic details; see [Yamatani-Saito, 2006].

Numerical Experiments



(a) JPEG, 23.61 dB

(b) FPHLCT, 24.19 dB

(c) PPHLCT, 23.97 dB

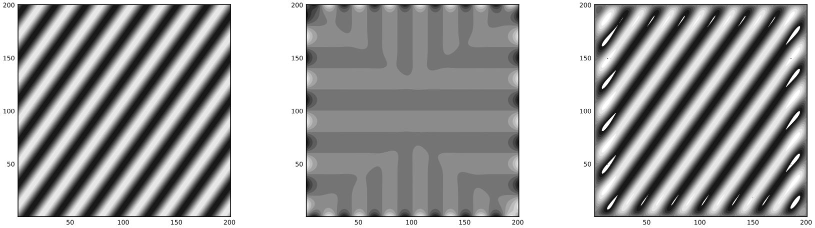
Figure: Compressed at 0.15 bits/pixel. Numerical values indicate the Peak Signal-to-Noise Ratio (PSNR) $:= 20\log_{10} \dfrac{\max_{(x,y)\in\Omega} |f(x,y)|}{\|f-\tilde{f}\|_2}$.

(a) JPEG, 25.67 dB (b) FPHLCT, 26.05 dB (c) PPHLCT, 25.73 dB

Figure: Compressed at 0.30 bits/pixel. Numerical values indicate the Peak Signal-to-Noise Ratio (PSNR).

Problems with Oscillatory Textures

- Solutions of the Laplace/Poisson equations *quickly attenuate oscillatory patterns* at the boundary when evaluated at the inside of the domain.
- This leads to inefficient $u+v$ decomposition for oscillatory patterns.



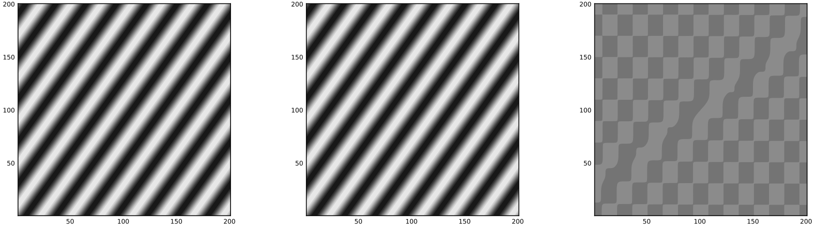
(a) Enemy f (b) Harmonic u (c) Residual v

Figure: The solution of Laplace's equation may lead to an inefficient $u+v$ decomposition.

Using the Helmholtz Equation for Oscillatory Textures

- The *Helmholtz* equation may rescue us:

$$\Delta u + k^2 u = 0 \quad \text{in } \Omega; \qquad \partial_\nu u = \partial_\nu f \quad \text{on } \partial\Omega.$$

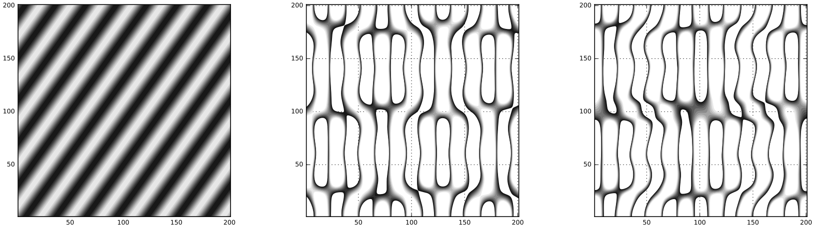


(a) Enemy f (b) Helmholtz u (c) Residual v

Figure: The Helmholtz equation may lead to an efficient $u+v$ decomposition.

Using the Helmholtz Equation for Oscillatory Textures . . .

- Important to use k (the wavenumber parameter) that should be estimated from the oscillatory patterns on $\partial\Omega$.



(a) Enemy f (b) Helmholtz u (c) Residual v

Figure: A wrong k may harm you.

Summary of Excursion I

- Both the FPHLCT and PPHLCT algorithms were *patented* as "Data Compression/Decompression Method, Program, and Device," Japan Patent # 4352110, Granted 8/7/09; US Patent # 8,059,903, Granted 11/15/11.
- More extensive numerical experiments (see [Yamatani-Saito 2006]) indicate that FPHLCT reduces the bit rates about 15% over JPEG whereas PPHLCT does about 7% to achieve the same PSNR in the relatively low bit rate range.
- PPHLCT is particularly useful because it accepts the files already compressed by the JPEG standard.
- Additional computational cost of both methods over JPEG is small: *linearly* proportional to the number of pixels of an input image.
- Using *the Helmholtz equation with the Neumann boundary condition* for u should be investigated! Any collaborations?
- In principle, the higher-order *polyharmonic operators* Δ^p, $p = 2, 3, \ldots$ can also be used instead of the Laplacian; however, the case $p > 2$ turned out to be impractical due to their requirement of higher-order boundary derivatives; see [Zhao-Saito-Wang, 2008] for the biharmonic ($p = 2$) version of PHL*S*T with the decay rate $O(\|\boldsymbol{k}\|^{-5})$.

My Heroes in Excursion I

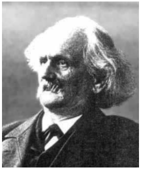
(a) P.-S. Laplace (1749–1827)

(b) J.B.J. Fourier (1768–1830)

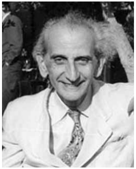
(c) S.D. Poisson (1781–1840)

(d) J.P.G.L. Dirichlet (1805–1859)

(e) H. von Helmholtz (1821–1894)



(f) Carl Neumann (1832–1925)



(g) Cornelius Lanczos (1893–1974)

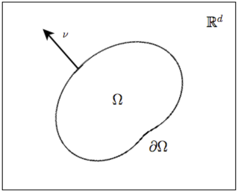
References for Excursion I

- K. Yamatani & N. Saito: "Improvement of DCT-based compression algorithms using Poisson's equation," *IEEE Trans. Image Process.*, vol.15, no.12, pp.3672–3689, 2006.
- N. Saito & J.-F. Remy: "The polyharmonic local sine transform: A new tool for local image analysis and synthesis without edge effect," *Appl. Comp. Harm. Anal.*, vol.20, no.1, pp.41–73, 2006.
- J. Zhao, N. Saito, & Y. Wang: "PHLST5: A practical and improved version of polyharmonic local sine transform," *J. Math. Imaging Vis.*, vo..30, pp.23–41, 2008.

Outline

Motivations

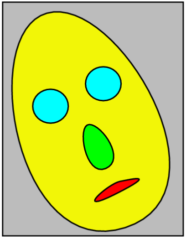
- Consider a bounded domain of general shape $\Omega \subset \mathbb{R}^d$.
- Want to analyze the spatial frequency information *inside* of the object defined in $\Omega \Longrightarrow$ need to avoid *the Gibbs phenomenon* due to $\partial\Omega$.
- Want to *represent* the object information efficiently for analysis, interpretation, discrimination, etc. $\Longrightarrow$ need *fast decaying* expansion coefficients relative to a *meaningful* basis.
- Want to extract and analyze *geometric information* about the domain $\Omega \Longrightarrow$ M. Kac: *"Can one hear the shape of a drum?"* (1966); spectral geometry; shape clustering/classification.



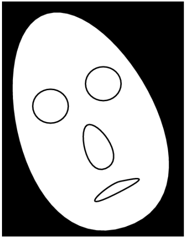
(a) $\Omega \subset \mathbb{R}^d$

(b) M. Kac (1914–1984)

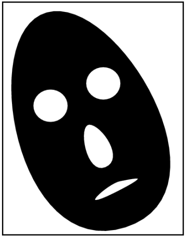
Object-Oriented Image Analysis



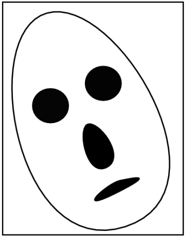
(a) Original



(b) Background

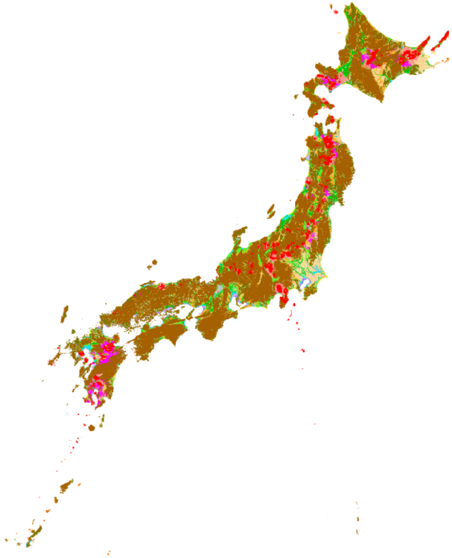


(c) Object

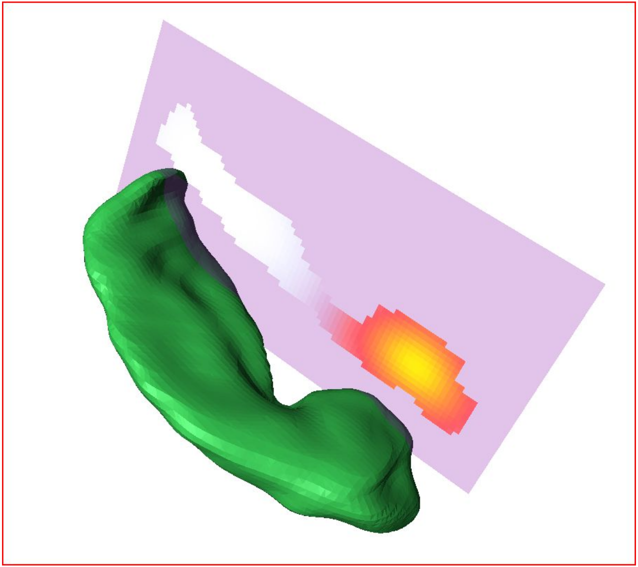


(d) Anomalies

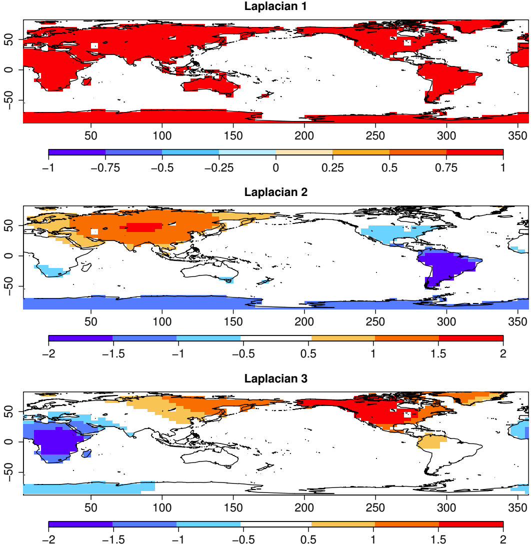
Data Analysis on a Complicated Domain



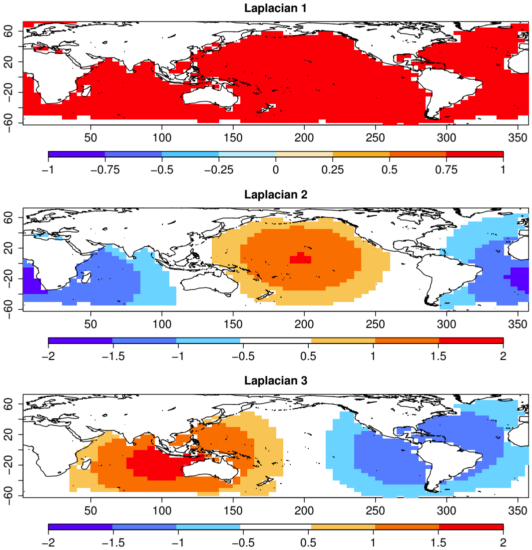
3D Hippocampus Shape Analysis (Courtesy: F. Beg)



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



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



Enter Laplacian Eigenfunctions!

- On 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 . . . 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!*
- The above statement needs to be interpreted very carefully due to the domain properties; e.g., quantum scars, LE localizations, . . .
  $\Longrightarrow$ see Excursion III.

Laplacian Eigenfunctions . . . Some Facts & 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.

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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

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

(a) G. Frobenius (1849–1917)

(b) B. Friedman (1915–1966)

- 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 2005, 2008)

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

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

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

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

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:*

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

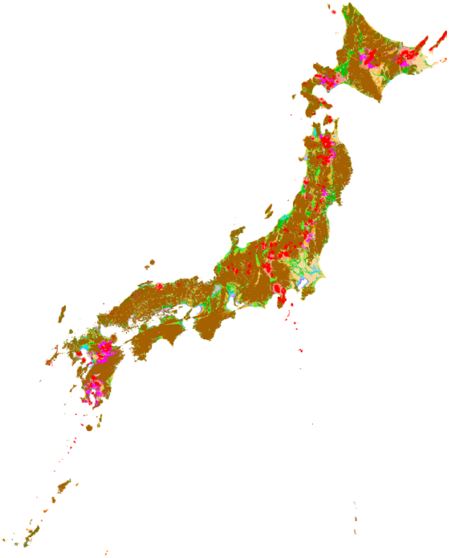
Corollary (NS 2005, 2008)

The integral operator $\mathcal{K}$ 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):*

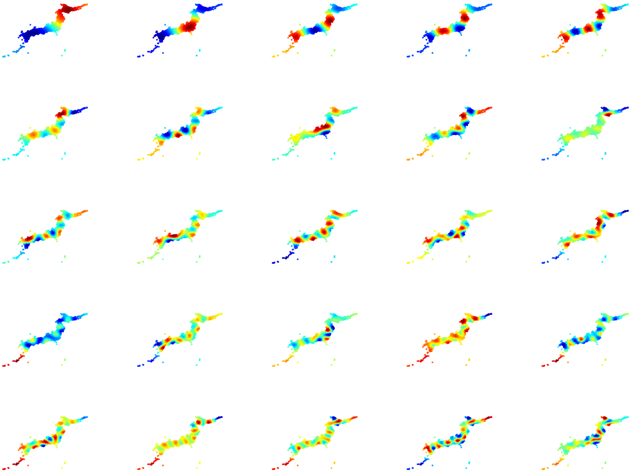
$$K(\boldsymbol{x}, \boldsymbol{y}) \sim \sum_{j=1}^{\infty} \mu_j \varphi_j(\boldsymbol{x}) \overline{\varphi_j(\boldsymbol{y})},$$

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

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



First 25 Basis Functions via the FMM-based algorithm



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.
- ...

Due to the time constraint, I will only talk about one application.

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- ...

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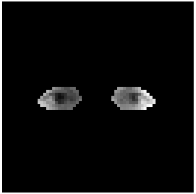
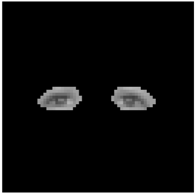
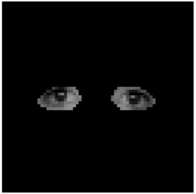
Statistical Image Analysis; Comparison with PCA

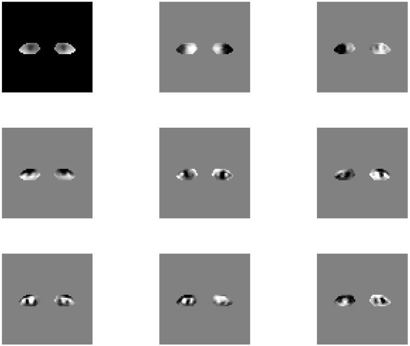
- Consider a stochastic process living on a domain Ω.
- *PCA/Karhunen-Loève Transform* is often used.
- PCA/KLT *implicitly* incorporate geometric information of the measurement (or pixel) location through *data correlation*.
- Our Laplacian eigenfunctions use *explicit* geometric information through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

Comparison with PCA: Example

- *"Rogue's Gallery"* dataset from Larry Sirovich
- Contains 143 faces
- Extracted left & right eye regions

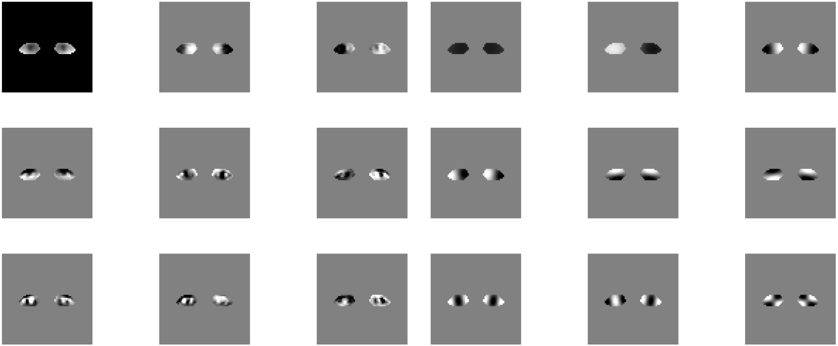




Comparison with PCA: Basis Vectors



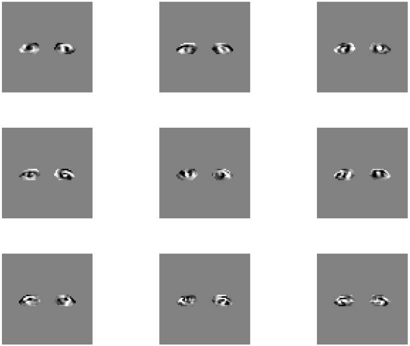
(a) KLB/PCA 1:9

Comparison with PCA: Basis Vectors

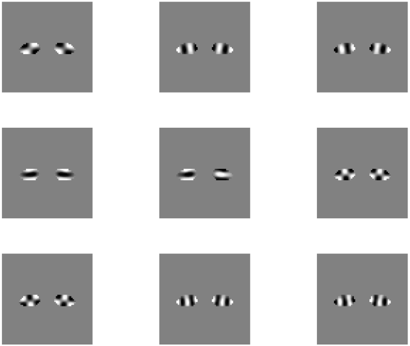


(a) KLB/PCA 1:9 (b) Laplacian Eigenfunctions 1:9

Comparison with PCA: Basis Vectors . . .

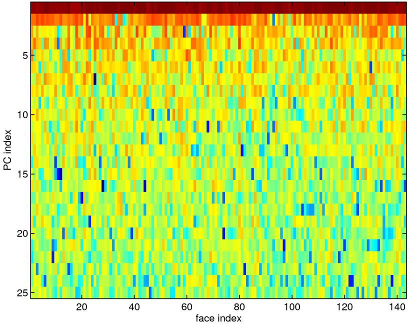


(a) KLB/PCA 10:18

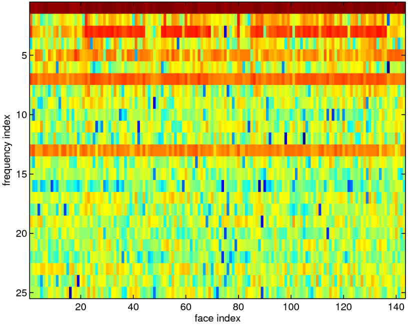


(b) Laplacian Eigenfunctions 10:18

Comparison with PCA: Energy Distribution over Coordinates

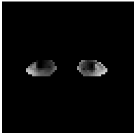


(a) KLB/PCA

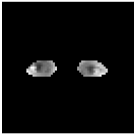


(b) Laplacian Eigenfunctions

Comparison with PCA: Basis Vector #7 . . .

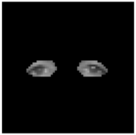


c_7:large

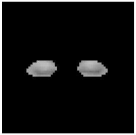


c_7:large

φ_7

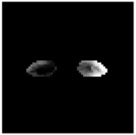


c_7:small

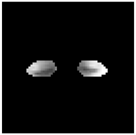


c_7:small

Comparison with PCA: Basis Vector #13 . . .



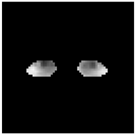
c_{13}:large



c_{13}:large

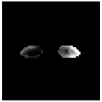
φ_{13}

c_{13}:small

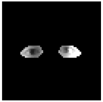


c_{13}:small

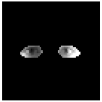
Asymmetry Detector



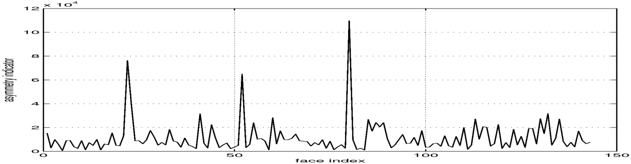
Eyes #80



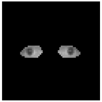
Eyes #22



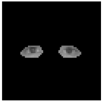
Eyes #52



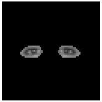
Asymmetry detector



Eyes #5



Eyes #84



Eyes #59

Summary of Excursion II

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 do:
  - Examine further our boundary conditions for specific geometry in higher dimensions; e.g., analysis on $\mathbb{S}^2$ 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 $(-\Delta)^p$, $p \geq 2$

My Heroes in Excursion II


(a) George Green (1793–1841)


(b) Lord Rayleigh (1842–1919)


(c) H.K.H. Weyl (1885–1955)


(d) J. von Neumann (1903–1957)


(e) Mark G. Kreĭn (1907–1989)


(f) M. Kac (1914–1984)


(g) V. Lidskiĭ (1924–2008)


(h) I. Gohberg (1928–2009)


(i) V. Rokhlin (1952–)


(j) L. Greengard (1958–)

References for Excursion II

- 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: "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*, accepted for publication, 2016.

Outline

Motivations: Why Graphs?

- More and more data are collected in a distributed and irregular manner; they are not organized such as familiar digital signals and images sampled on regular lattices. Examples include:
  - Data from sensor networks
  - Data from social networks, webpages, ...
  - Data from biological networks
  - ...
- It is quite important to analyze:
  - *Topology* of graphs/networks (e.g., how nodes are connected, etc.)
  - *Data* measured on nodes (e.g., a node = a sensor, then what is an edge?)

- *Fourier/wavelet analysis/synthesis* have been 'crown jewels' for data sampled on the regular lattices.
- Hence, we need to lift such tools for unorganized and irregularly-sampled datasets including those represented by graphs and networks.
- Moreover, constructing a graph from a usual signal or image and analyzing it can also be very useful!

An Example of Social Networks

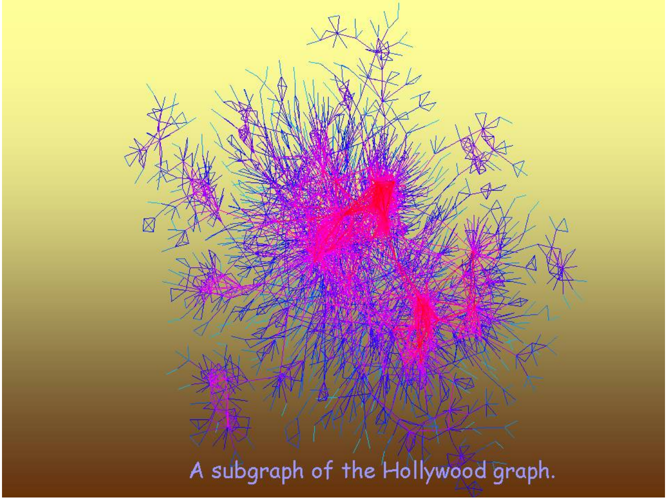
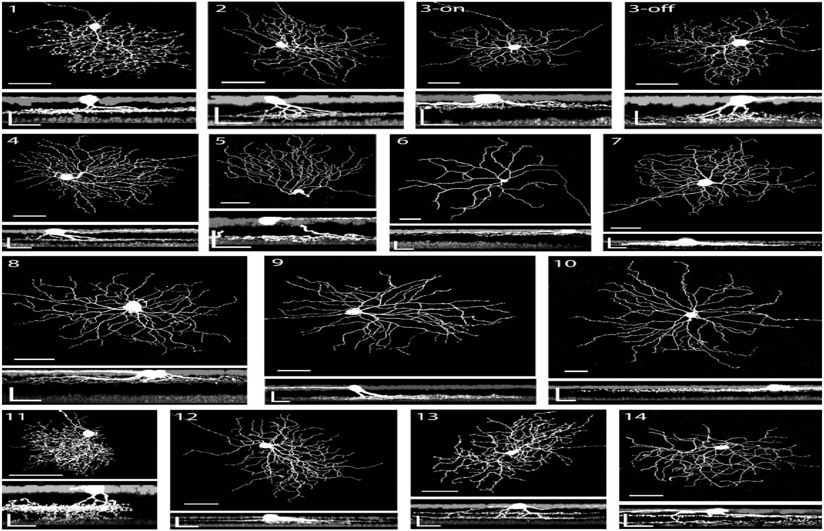
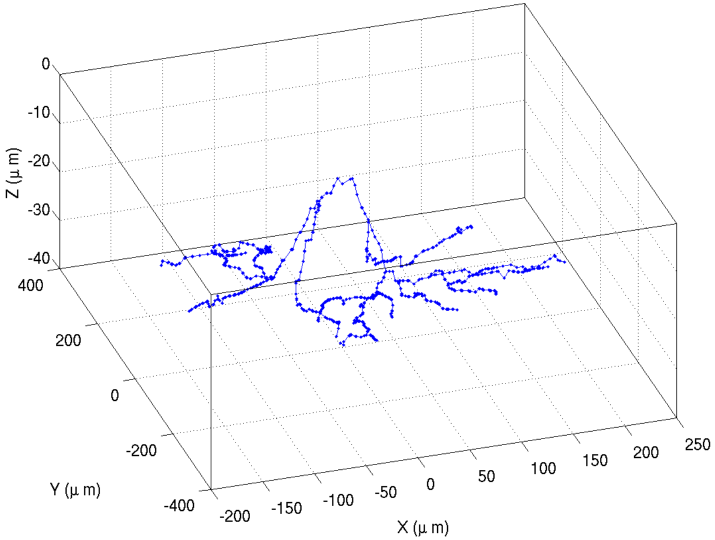


Figure: Through the courtesy of Prof. Fan Chung, UC San Diego

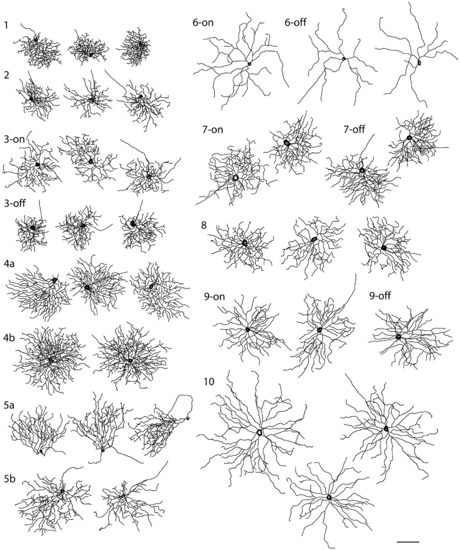
A Biological Example: Retinal Ganglion Cells



Mouse's RGC as a Graph



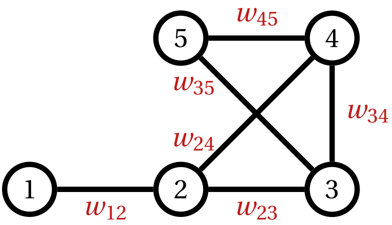
Can we hear the shape of dendritic trees?



Definitions and Notation

Let G be an *undirected graph*.

- $V = V(G) = \{v_1, \ldots, v_n\}$ is the set of *vertices* (or *nodes*).
- For simplicity, we often use $1, \ldots, n$ instead of $v_1, \ldots, v_n$.
- $E = E(G) = \{e_1, \ldots, e_m\}$ is the set of *edges*, where $e_k = (i, j)$ represents an edge (or line segment) connecting between adjacent vertices i, j for some $1 \le i, j \le n$.
- $W = W(G) \in \mathbb{R}^{n \times n}$ is the *weight matrix*, where w_{ij} denotes the edge weight between vertices i and j.



Matrices Associated with a Graph

- The *adjacency matrix* $W = W(G) = (w_{ij}) \in \mathbb{R}^{n \times n}$, $n = |V|$, for an unweighted graph G consists of the following entries:

$$w_{ij} := \begin{cases} 1 & \text{if } i \sim j; \\ 0 & \text{otherwise.} \end{cases}$$

- Another typical way to define its entries is based on the *similarity* of information at nodes i and j:

$$w_{ij} := \exp(-\mathrm{dist}(i,j)^2/\epsilon^2)$$

where $\mathrm{dist}(\cdot,\cdot)$ is an appropriate distance measure (i.e., metric) defined in V, and $\epsilon > 0$ is an appropriate scale parameter. This leads to a *weighted* graph.

Matrices Associated with a Graph ...

- The *degree matrix* $D = D(G) = \mathrm{diag}(d_1, \ldots, d_n) \in \mathbb{R}^{n \times n}$ is a diagonal matrix whose entries are:

$$d_i := \sum_{j=1}^{n} w_{ij}.$$

  Note that the above definition works for both unweighted and weighted graphs.

- The *transition matrix* $P = P(G) = (p_{ij}) \in \mathbb{R}^{n \times n}$ consists of the following entries:

$$p_{ij} := w_{ij}/d_i \quad \text{if } d_i \neq 0.$$

- p_{ij} represents the probability of a random walk from i to j in one step: $\sum_j p_{ij} = 1$, i.e., P is *row stochastic*.
- $W^{\mathsf{T}} = W$, $P^{\mathsf{T}} \neq P$, $P = D^{-1} W$.

Matrices Associated with a Graph ...

- Let G be an *undirected* graph. Then, we can define several *Laplacian* matrices of G:

$$L(G) := D - W \qquad \textit{Unnormalized}$$

$$L_{\mathrm{rw}}(G) := I_n - D^{-1}W = I_n - P = D^{-1}L \qquad \textit{Normalized}$$

$$L_{\mathrm{sym}}(G) := I_n - D^{-\frac{1}{2}}WD^{-\frac{1}{2}} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}} \qquad \textit{Symmetrically-Normalized}$$

- Graph Laplacians can also be defined for *directed* graphs; However, there are many different definitions based on the types/classes of directed graphs, and in general, those matrices are *nonsymmetric*.

Functions/Vectors Defined on a Graph

- Let $f \in \mathcal{L}^2(V) \equiv \mathbb{R}^n$. Then

$$(Lf)_i = d_i f_i - \sum_{j=1}^{n} w_{ij} f_j = \sum_{j=1}^{n} w_{ij} \left(f_i - f_j\right).$$

  i.e., this is a generalization of the *finite difference approximation* to the Laplace operator.

- On the other hand,

$$(L_{\mathrm{rw}} f)_i = f_i - \sum_{j=1}^{n} p_{ij} f_j = \frac{1}{d_i} \sum_{j=1}^{n} w_{ij} \left(f_i - f_j\right).$$

$$(L_{\mathrm{sym}} f)_i = f_i - \frac{1}{\sqrt{d_i}} \sum_{j=1}^{n} \frac{w_{ij}}{\sqrt{d_j}} f_j = \frac{1}{\sqrt{d_i}} \sum_{j=1}^{n} w_{ij} \left(\frac{f_i}{\sqrt{d_i}} - \frac{f_j}{\sqrt{d_j}} \right).$$

- Note that these definitions of the graph Laplacian corresponds to $-\Delta$ in $\mathbb{R}^d$, i.e., they are *nonnegative operators* (a.k.a. *positive semi-definite matrices*).

Why Graph Laplacians?

- We already know the usefulness of Laplacian eigenvalues and eigenfunctions for general domains in $\mathbb{R}^d$ via Excursion II.
- The graph Laplacian *eigenvalues* reflect various intrinsic geometric and topological information about the graph including connectivity or the number of separated components; diameter; mean distance, . . .
- Fan Chung: *Spectral Graph Theory*, Amer. Math. Soc., 1997, says: *"This monograph is an intertwined tale of eigenvalues and their use in unlocking a thousand secrets about graphs."*

Why Graph Laplacian Eigenfunctions?

- The graph Laplacian *eigenfunctions* form an *orthonormal basis* on a graph $\Longrightarrow$
  - can *expand* functions defined on a graph
  - can perform *spectral analysis/synthesis/filtering* of data measured on vertices of a graph
- Can be used for graph partitioning, graph drawing, data analysis, clustering, ... $\Longrightarrow$ *Graph Cut*, *Spectral Clustering*, which can be viewed as an application of the discrete version of *the Courant Nordal Domain Theorem*.
- Less studied than graph Laplacian eigenvalues
- In this talk, I will use the terms "eigenfunctions" and "eigenvectors" interchangeably.
- Also, an eigenvector/function is denoted by $\boldsymbol{\phi}$, and its value at vertex $x \in V$ is denoted by $\boldsymbol{\phi}(x)$.

A Simple Yet Important Example: A Path Graph

$$\underbrace{\begin{bmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{bmatrix}}_{L(G)} = \underbrace{\begin{bmatrix} 1 & & & & & \\ & 2 & & & & \\ & & 2 & & & \\ & & & \ddots & & \\ & & & & 2 & \\ & & & & & 1 \end{bmatrix}}_{D(G)} - \underbrace{\begin{bmatrix} 0 & 1 & & & & \\ 1 & 0 & 1 & & & \\ & 1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & 0 & 1 \\ & & & & 1 & 0 \end{bmatrix}}_{W(G)}$$

The eigenvectors of this matrix are exactly the *DCT Type II* basis vectors used for the JPEG image compression standard! (See G. Strang, "The discrete cosine transform," *SIAM Review*, vol. 41, pp. 135–147, 1999).

- $\lambda_k = 2 - 2\cos(\pi k/n) = 4\sin^2(\pi k/2n),\ k = 0, 1, \ldots, n-1.$
- $\boldsymbol{\phi}_k(\ell) = \cos\left(\pi k\left(\ell + \frac{1}{2}\right)/n\right),\ k, \ell = 0, 1, \ldots, n-1.$
- In this simple case, λ (eigenvalue) is a monotonic function w.r.t. the frequency, which is the eigenvalue index k. *For a general graph, however, the notion of frequency is not well defined.*

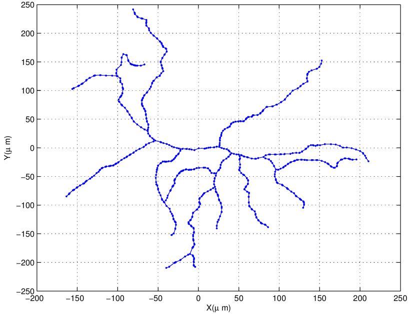
A Brief Review of Graph Laplacian Eigenvalues

- In this review part, we only consider *undirected* and *unweighted* graphs and their *unnormalized* Laplacians $L(G) = D(G) - W(G)$. Let $|V(G)| = n$, $|E(G)| = m$.
- It is a good exercise to see how the statements change for L_{rw}, L_{sym}.
- Can show that $L(G)$ is *positive semi-definite*.
- Hence, we can *sort* the eigenvalues of $L(G)$ as $0 = \lambda_0(G) \le \lambda_1(G) \le \cdots \le \lambda_{n-1}(G)$ and denote the set of these eigenvalue by $\Lambda(G)$.
- $m_G(\lambda) :=$ the multiplicity of λ.
- Let $I \subset \mathbb{R}$ be an interval of the real line. Then define $m_G(I) := \#\{\lambda_k(G) \in I\}$.

- Graph Laplacian matrices of the same graph are *permutation-similar*. In fact, graphs G_1 and G_2 are *isomorphic* iff there exists a permutation matrix Q such that
$$L(G_2) = Q^{\mathsf{T}} L(G_1) Q.$$
- $\operatorname{rank} L(G) = n - m_G(0)$ where *$m_G(0)$ turns out to be the number of connected components of G*. Easy to check that $L(G)$ becomes $m_G(0)$ diagonal blocks.
- The eigenspace corresponding to the zero eigenvalues is spanned by the *indicator* vectors of each connected component, which are called the *Perron* vectors due to *the Perron-Frobenius Theorem*.
- In particular, $\lambda_1 \neq 0$, i.e., $m_G(0) = 1$ iff G is connected.
- This led M. Fiedler (1973) to define the *algebraic connectivity* of G by $a(G) := \lambda_1(G)$, viewing it as a *quantitative measure of connectivity*.
- The corresponding eigenvector is called the *Fiedler* vector, which is used to bipartition G.

A Peculiar Phase Transition Phenomenon

We observed an interesting phase transition phenomenon on the behavior of the eigenvalues of *graph Laplacians* defined on dendritic trees.



(a) RGC #100

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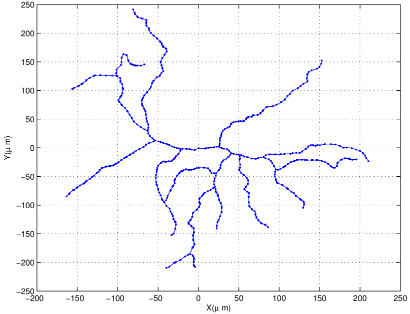
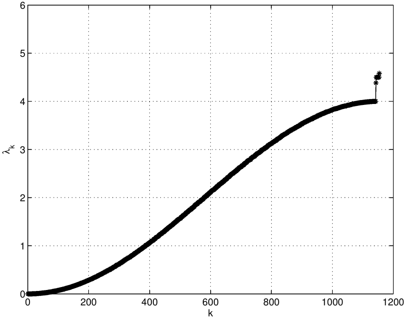


(a) RGC #100



(b) Eigenvalues of RGC #100

A Peculiar Phase Transition Phenomenon . . .

We have observed that this value 4 is critical since:

- the eigenfunctions corresponding to the eigenvalues below 4 are *semi-global oscillations* (like *Fourier cosines/sines*) over the entire dendrites or one of the dendrite arbors;
- those corresponding to the eigenvalues above 4 are much more *localized* (like *wavelets*) around *junctions/bifurcation vertices*.

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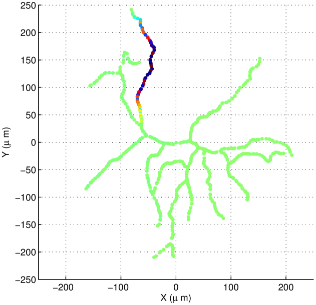

(a) RGC #100; $\lambda_{1141} = 3.9994$

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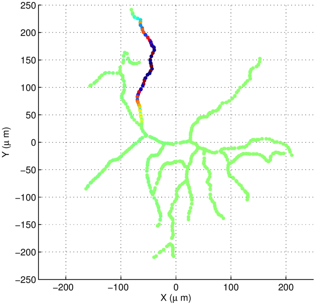

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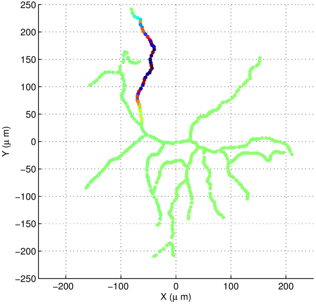

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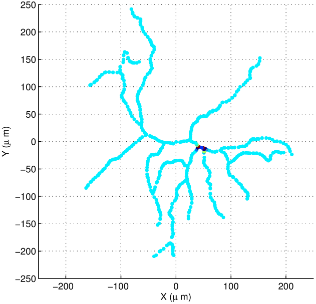
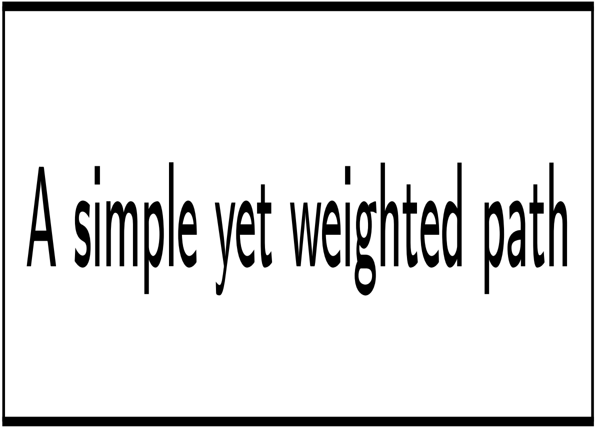


(b) RGC #100; $\lambda_{1142} = 4.3829$

- We know why such localization/phase transition occurs $\Longrightarrow$ See our article for the detail: Y. Nakatsukasa, N. Saito, & E. Woei: "Mysteries around graph Laplacian eigenvalue 4," *Linear Algebra & Its Applications*, vol. 438, no. 8, pp. 3231–3246, 2013. The key was the *discriminant* of a quadratic equation.
- Any physiological consequence? Importance of branching vertices?
- Many such eigenvector localization phenomena have been reported: Anderson localization, scars in quantum chaos, ...
- See also an interesting related work for more general setting and for application in numerical linear algebra: I. Krishtal, T. Strohmer, & T. Wertz: "Localization of matrix factorizations," *Foundations of Comp. Math.*, vol. 15, no. 4, pp. 931–951, 2015.
- Our point is that *eigenvectors corresponding to high eigenvalues are quite sensitive to topology and geometry of the underlying domain and cannot really be viewed as high frequency oscillations unless the underlying graph is a simple unweighted path or cycle.*
- Hence, one must be very careful to develop an analog of *the Littlewood-Paley theory* for general graphs!

- Even on a simple path, if edges are unequally weighted, localization can occur!



Play/Pause

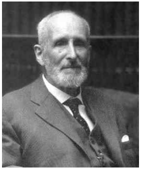
- We want to control such eigenvector localizations by ourselves rather than dictated by the topology and geometry of the graphs!
- This led us to the development of the *multiscale basis dictionaries* on graphs; see my papers with Jeff Irion and the 2016 newsletter of our department.

Summary of Excursion III

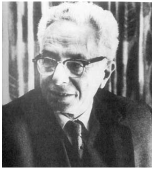
- Laplacian *eigenfunctions* can be nicely defined on a graph G.
- They allow us to perform *spectral analysis* of data recorded on $V(G)$.
- However, these eigenfunctions reveal nontrivial traits (e.g., localization) depending on topology and edge weights of G.
- Hence, one can*not* make exact parallel analogy between the Laplacian eigenbasis and the Fourier basis unless G is a path or a cycle.
- What about integral operators commuting with graph Laplacian matrices? $\Longrightarrow$ some functions of the *distance matrix* of G seem like good candidates
- Lots of things to do: analysis of *directed graphs*; dealing with *graph connection Laplacian* (e.g., edge weights are group transformations while vertices represent transformed images); further development of *wavelet packet basis dictionaries on matrices and tensors*; ...

My Heroes/Heroine in Excursion III

(a) F.G. Frobenius (1849–1917)



(b) Oskar Perron (1880–1975)



(c) Richard Courant (1888–1972)

(d) Miroslav Fiedler (1926–2015)

(e) Hajime Urakawa (1946–)

(f) Fan R.K. Chung Graham (1949–)

References for Excursion III

- My MAT 280 Course Slides on "Harmonic Analysis on Graphs and Networks"
- N. Saito & E. Woei: "Analysis of neuronal dendrite patterns using eigenvalues of graph Laplacians," *Japan SIAM Letters*, vol. 1, pp. 13–16, 2009.
- N. Saito & E. Woei: "On the phase transition phenomenon of graph Laplacian eigenfunctions on trees," *RIMS Kôkyûroku*, vol. 1743, pp. 77–90, 2011.
- Y. Nakatsukasa, N. Saito, & E. Woei: "Mysteries around graph Laplacian eigenvalue 4," *Linear Algebra & Its Applications*, vol. 438, no. 8, pp. 3231–3246, 2013.
- J. Irion & N. Saito: "Hierarchical graph Laplacian eigen transforms," *JSIAM Letters*, vol. 6, pp. 21–24, 2014.
- J. Irion & N. Saito: "The generalized Haar-Walsh transform," *Proc. 2014 IEEE Workshop on Statistical Signal Processing*, pp. 488–491, 2014.
- J. Irion & N. Saito: "Applied and computational harmonic analysis on graphs and networks," in *Wavelets and Sparsity XVI, Proc. SPIE 9597*, Paper # 95971F, 2015.
- J. Irion & N. Saito: "Efficient approximation and denoising of graph signals using the multiscale basis dictionaries," *IEEE Trans. Signal and Inform. Process. Netw.*, accepted for publication, 2016.

Outline

Overall Summary

- Through my own work and effort, I realized how right Prof. Urakawa was about his impression on the proverb *"There is good mathematics around Laplacians."*
- Laplacians are connected to lots of interesting mathematics: Fourier analysis, spectral geometry, spectral graph theory, isoperimetric inequalities, Toeplitz operators, PDEs, potential theory, stochastic processes, almost-periodic functions, ...
- Laplacians are also useful and being used in many applications!
- *How to naturally order/sort Laplacian eigenfunctions?* $\Longrightarrow$ Not by the size of the corresponding eigenvalues, but by something else!
- Want to study more about Laplacians on *manifolds*, i.e., Laplace-Beltrami operators!

Thank you very much for your attention!

This talk is dedicated to my four mentors:


(a) Yves F. Meyer (1939–)


(b) Ronald R. Coifman (1941–)


(c) Gregory Beylkin (1953–)


(d) David L. Donoho (1957–)