Accessing geometry via function spaces

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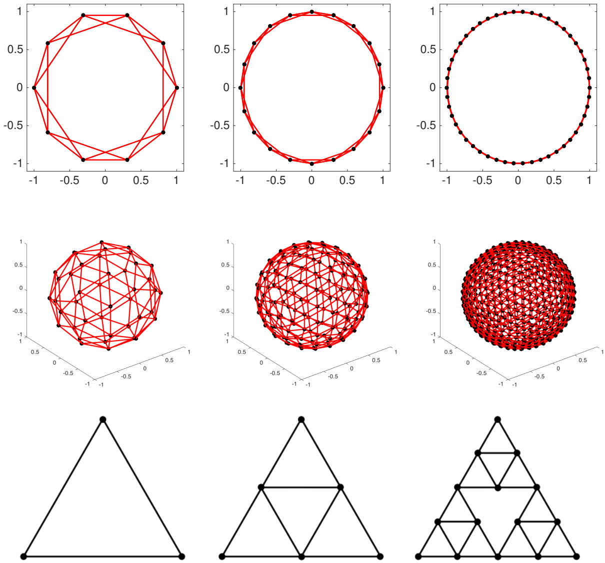
ROADMAP

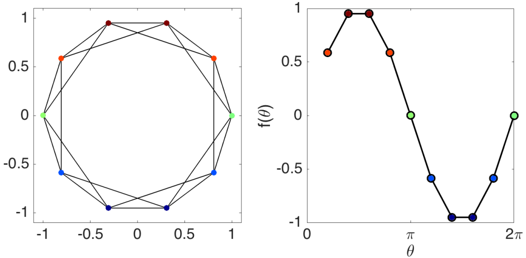
- Limits of graphs
- Geometric objects of interest:
  - Intrinsic distances
  - Symmetries
- Why function spaces?
  - Visualization
  - Finding symmetries
  - Algebras on function space

LIMITS OF GRAPHS



DISCRETE FUNCTION SPACES

- Sequence of graphs (V_n, E_n) approximating $\Omega \supset V_n$
- Define function spaces $\ell(V_n) = \{f : V_n \to \mathbb{R}\}$
  - $\ell(V_n) \cong \mathbb{R}^N$ (where N is size of V_n) by $\vec{f}_i = f(x_i)$
  - Inner product $f \cdot h = \sum_{x \in V_n} f(x)h(x)$
  - Restriction of $f : \Omega \to \mathbb{R}$ by $\Pi_n f = f|_{V_n}$



1	0.5878
2	0.9511
3	0.9511
4	0.5878
5	0
6	-0.5878
7	-0.9511
8	-0.9511
9	-0.5878
10	0

WHY FUNCTION SPACES?

- Sequence of graphs (V_n, E_n) approximating $\Omega \supset V_n$
- Hard to define limit $(V_n, E_n) \to \Omega$
- Assume $V_n \subset V_{n+1}$ and $V^* = \bigcup_n V_n$ dense in Ω
- Easy to define limit $f_n \to f$ by $||f_n - \Pi_n f|| \to 0$
- Requires some assumptions on f, e.g. smoothness
- Convergence of functions doesn't tell us about geometry
- We need operators! Haven't used the edges yet....

GRAPH LAPLACIANS

- Build a random walk
  - Assign weights to edges $\mathbf{K}_{ij} \geq 0$ for $i \sim j$
  - Compute row sums $\mathbf{D}_{ii} = \sum_j \mathbf{K}_{ij}$
  - Divide rows by row sums $\mathbf{P} = \mathbf{D}^{-1}\mathbf{K}$
  - $\mathbf{P}$ is a Markov matrix (transition probabilities)
- Assume symmetric $\mathbf{K}_{ij} = \mathbf{K}_{ji}$ non-negative def. $\vec{v}^\top \mathbf{K}\vec{v} \geq 0$
- Define the associated graph Laplacian $\mathbf{L} = \mathbf{P} - \mathbf{I}$
- $\mathbf{L}$ is called the generator of the random walk

DISCRETE ANALOGS OF CONTINUOUS OBJECTS

Continuous	Discrete
$L^2(\Omega)$	$\mathbb{R}^N$
Functions, $f : \mathcal{M} \to \mathbb{R}$	Vectors, $\vec{f}_i = f(x_i)$
'Basis', δ_x	Basis, $\vec{e}_i = \delta_{x_i}$
Operators, $\mathcal{F}$	Matrices, $\mathbf{F}$
Laplacian, Δ	graph Laplacian, $\mathbf{L}$
Eigenfunctions, $\Delta\varphi_j = \lambda_j\varphi_j$	Eigenvectors, $\mathbf{L}\vec{\varphi}_j = \lambda_j\vec{\varphi}_j$
Inner product, $\langle f, h\rangle_{L^2}$	Dot Product, $\vec{f} \cdot \vec{h}$
Measure, $\langle f, h\rangle_{L^2, d\mu}$	Diagonal matrix, $\vec{f} \cdot_D \vec{h} = \vec{f}^\top D\vec{h}$

Limits of Graph Laplacians

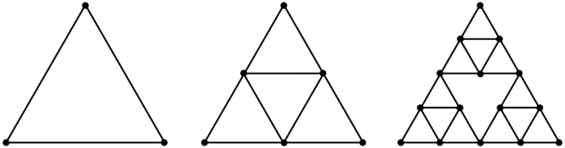
- Sequence of graphs (V_n, E_n) approximating $\Omega \supset V_n$
- Define a sequence graph Laplacians $\mathbf{L}_n = \mathbf{P}_n - \mathbf{I}$
- Find scaling factors c_n such that $c_n \mathbf{L}_n$ converges pointwise

$$c_n \mathbf{L}_n \vec{f} \to \mathcal{L} f$$

- Meaning that for nice functions $f : \Omega \to \mathbb{R}$

$$\lim_{n\to\infty} ||c_n \mathbf{L}_n \Pi_n f - \Pi_n \mathcal{L} f|| = 0$$

EXAMPLE 1: LAPLACIANS ON FRACTALS

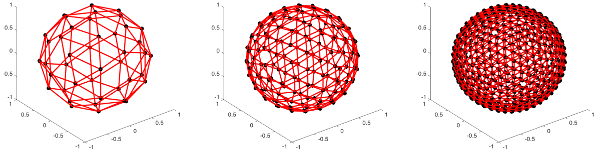


- Sequence of graphs (V_n, E_n) approximating $\Omega \supset V_n$
- Uniform random walk $K_{ij} = 1$ if $i \sim j$
- For the Sierpinski gasket (SG, shown above) $c_n = 5^n$

$$c_n \mathbf{L}_n \vec{f}_i = 5^n \sum_{j \sim i \text{ in } V_n} \big(f(x_j) - f(x_i)\big) \to \Delta f$$

- Δ is the foundation of analysis on SG

EXAMPLE 2: LAPLACIANS ON MANIFOLDS



- Sequence of graphs (V_n, E_n) approximating $\Omega \supset V_n$
- Local random walk $K_{ij} = \exp\left(-\frac{||x_i - x_j||^2}{4\delta^2}\right)$
- For d-dimensional manifold $c_n = \delta^{-2}$ where $\delta = N^{-\frac{1}{6+d}}$

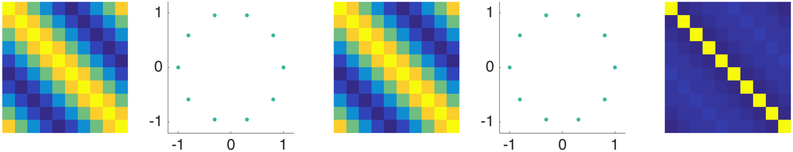
$$c_n \mathbf{L}_n \vec{f}_i \to \Delta f$$

- Δ is the Laplace-Beltrami operator

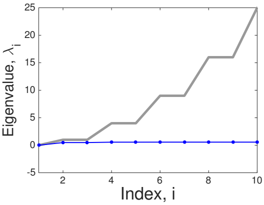
LAPLACIAN ON S^1, 10 POINTS

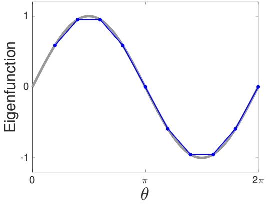
Parameterize $S^1 = \{\theta \in [0, 2\pi)\}$, Laplacian is $\Delta = -\frac{d^2}{d\theta^2}$

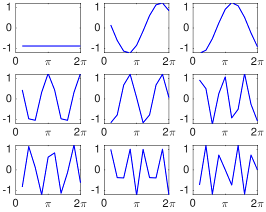
Kernel | Density | Normalized | Bias | Laplacian



K | $D = K1$ | $\hat{K} = D^{-1}KD^{-1}$ | $\hat{D} = \hat{K}1$ | L



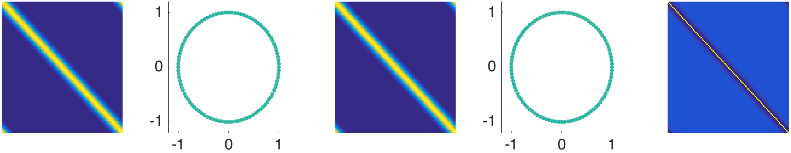




LAPLACIAN ON S^1, 100 POINTS

Parameterize $S^1 = \{\theta \in [0, 2\pi)\}$, Laplacian is $\Delta = -\frac{d^2}{d\theta^2}$

Kernel | Density | Normalized | Bias | Laplacian



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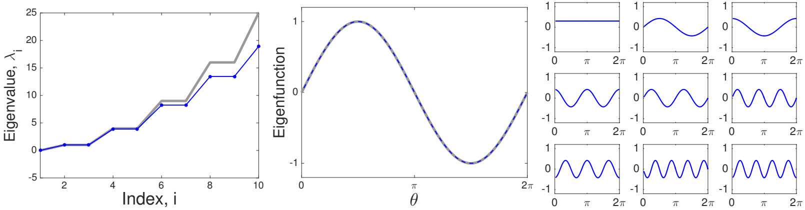
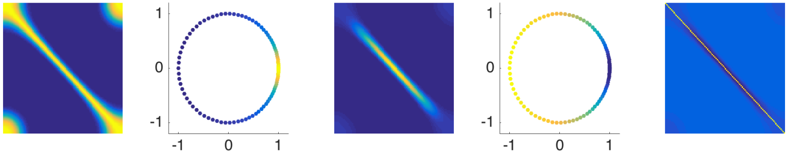


NONUNIFORM S^1, 100 POINTS

Parameterize $S^1 = \{\theta \in [0, 2\pi)\}$, Laplacian is $\Delta = -\frac{d^2}{d\theta^2}$

Kernel	Density	Normalized	Bias	Laplacian



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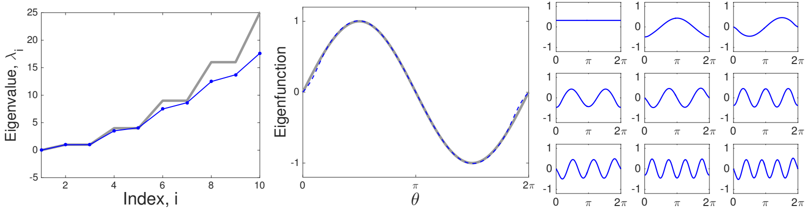
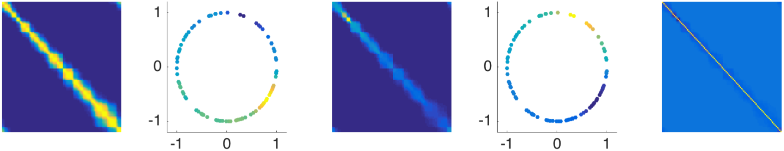


Real Data S^1, 100 points

Parameterize $S^1 = \{\theta \in [0, 2\pi)\}$, Laplacian is $\Delta = -\frac{d^2}{d\theta^2}$

Kernel	Density	Normalized	Bias	Laplacian



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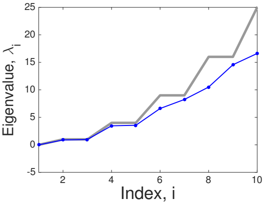
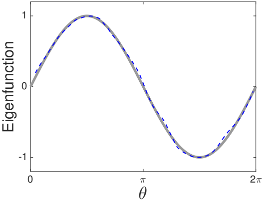
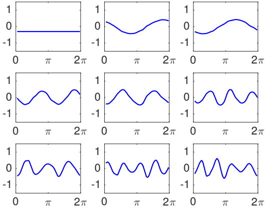


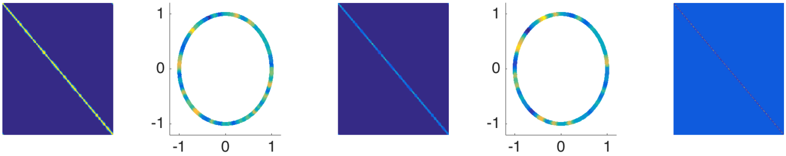




REAL DATA S^1, 1000 POINTS

Parameterize $S^1 = \{\theta \in [0, 2\pi)\}$, Laplacian is $\Delta = -\frac{d^2}{d\theta^2}$

Kernel	Density	Normalized	Bias	Laplacian



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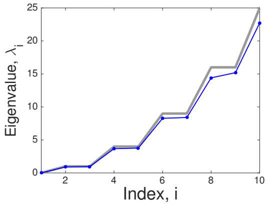
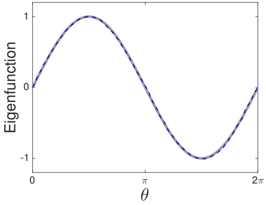
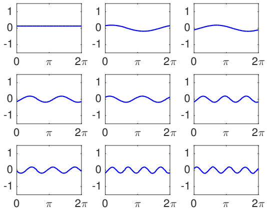






LESSON LEARNED SO FAR...

- We can approximate manifolds/fractals by graphs
- Nice convergence notions on functions/operators
- Graph Laplacians converge to continuous Laplacians
- Sampling is important!

A BIT OF RIEMANNIAN GEOMETRY

- Consider a smooth d-dimensional manifold $\mathcal{M}$
- There is no canonical inner product on tangent spaces
- A Riemannian metric g is a choice of inner product

$$g_x : T_x\mathcal{M} \times T_x\mathcal{M} \to \mathbb{R}$$

- g_x is bilinear, symmetric, positive definite, and smooth in x
- **Example:** Let $\iota : \mathcal{M} \to \mathbb{R}^m$ be a smooth embedding

$$g_x(v, w) = \langle D\iota(x)v, D\iota(x)w \rangle_{\mathbb{R}^m}$$

- g is called the induced metric

RIEMANNIAN VOLUME

- Choose coordinates $x^1, ..., x^d : U_x \to \mathbb{R}$
- Basis vectors $e_1, ..., e_d \in T_x\mathcal{M}$ where $e_i = \frac{\partial}{\partial x^i}$
- Represent g_x as a matrix $g_{ij}(x) = g_x(e_i, e_j)$
- Define the volume form $dV(x) = \sqrt{\det(g(x))}\, dx^1 \cdots dx^d$
- $\mathrm{vol}(\mathcal{M}) = \int_{x\in\mathcal{M}} 1\, dV(x)$
- Now we can define a nice function space $L^2(\mathcal{M}, g)$

WHY IS THE RIEMANNIAN METRIC A GEOMETRY?

- Allows us to measure tangent vectors $||v||_g^2 = g_x(v, v)$
- Given a differentiable curve $\gamma : [0, 1] \to \mathcal{M}$ we can define the length, $L(\gamma) \equiv \int_0^1 ||\gamma'(t)||dt$
- We define the intrinsic distance $d_{\mathcal{I}}(x, y) \equiv \inf_\gamma L(\gamma)$
- If some γ attains $d_{\mathcal{I}}(x, y)$ it is a geodesic
- $(\mathcal{M}, d_{\mathcal{I}})$ is called a *path metric space*

WHAT ARE ISOMETRIES?

- Let $\mathcal{T} : \mathcal{M} \to \mathcal{N}$ be a diffeomorphism
- We call $\mathcal{T}$ an isometry if $g_{\mathcal{M}} = \mathcal{T}^* g_{\mathcal{N}}$
  - Pick orthonormal bases $v_1, ..., v_d \in T_x\mathcal{M}$ and $w_1, ..., w_d \in T_{\mathcal{T}(x)}\mathcal{N}$
  - Represent $D\mathcal{T}(x) : T_x\mathcal{M} \to T_{\mathcal{T}(x)}\mathcal{N}$ in these bases
  - $\mathcal{T}$ is an isometry if $D\mathcal{T}(x)$ is an orthogonal matrix
- $\mathcal{T}$ is an isometry $\Leftrightarrow d_{\mathcal{I},\mathcal{M}}(x, y) = d_{\mathcal{I},\mathcal{N}}(\mathcal{T}(x), \mathcal{T}(y))$
- $\Leftarrow$ is Myers-Steenrod theorem (proves $\mathcal{T}$ is diffeo)

ISOMETRIES AND THE LAPLACIAN

- Isometries $\mathcal{T} : \mathcal{M} \to \mathcal{N}$ preserve the metric, g
- Laplacian is defined by g

$$\Delta f = \text{div} \circ \nabla = \frac{1}{\sqrt{|g|}} \partial_i g^{ij} \sqrt{|g|} \partial_j f$$

- Laplacian is preserved by isometries

$$\Delta_{\mathcal{N}}(f \circ \mathcal{T}) = \Delta_{\mathcal{M}}(f) \circ \mathcal{T}$$

Visualization: Diffusion maps

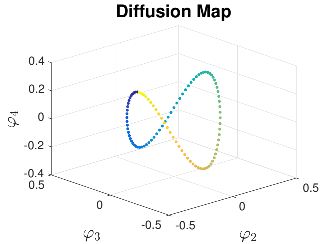
- Eigenfunctions $\Delta\varphi_j = \lambda_j \varphi_j$ define isometric embedding

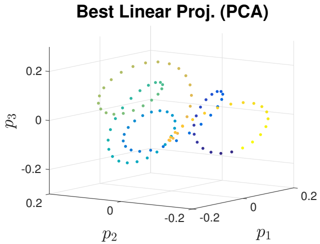
$$\Phi : x \mapsto c(e^{-\lambda_1 t}\varphi_1(x), e^{-\lambda_2 t}\varphi_2(x), \ldots)$$

- Embed $S^1 \subset \mathbb{R}^6$ by

$$t \mapsto (\cos(t), \sin(t), \cos(2t), \sin(2t), \cos(5t), \sin(5t))/\sqrt{30}$$

- Want to project back to $\mathbb{R}^3$





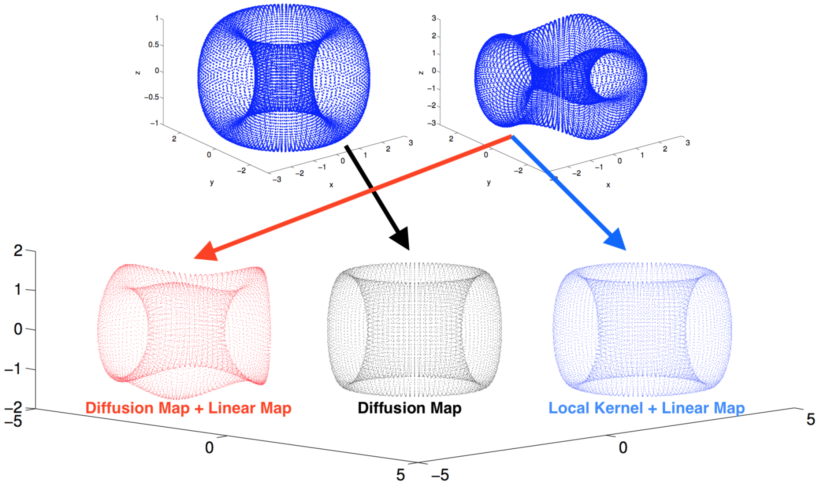
LEARNING NONLINEAR MAPS

- Assume we have two data sets $\{x_i\}_{i=1}^N$ and $\{y_i\}_{i=1}^N$
- Related by a diffeomorphism $y_i = \mathcal{H}(x_i)$

$$\begin{array}{ccc} \mathcal{M} & \xrightarrow{\mathcal{H}} & \mathcal{H}(\mathcal{M}) \\ \Big\downarrow \tilde{\Phi} & & \Big\downarrow \Phi \\ \ell^2 \cong L^2(\mathcal{M}, \tilde{g}) & \xrightarrow{U} & \ell^2 \cong L^2(\mathcal{H}(\mathcal{M}), g) \end{array}$$

- $\tilde{\Phi}$ and Φ are built with Local Kernels
- U is orthogonal linear map $\Rightarrow$ Easy to fit

LEARNING NONLINEAR MAPS



WHAT ARE SYMMETRIES?

- Isometries preserve the Riemannian metric, g, and the intrinsic distance, $d_{\mathcal{I}}$
- Consider isometries $\mathcal{T} : \mathcal{M} \to \mathcal{M}$
- Group structure: Composition of isometries is an isometry
- Laplacian is preserved $\Delta(f \circ \mathcal{T}) = \Delta(f) \circ \mathcal{T}$
- Hard Theorem: Isometries form a Lie group

SYMMETRIES AND EIGENFUNCTIONS

- Consider an non-trivial isometry $\mathcal{T} : \mathcal{M} \to \mathcal{M}$
- Consider an eigenfunction $\Delta\varphi_j = \lambda_j\varphi_j$

$$\Delta(\varphi_j \circ \mathcal{T}) = \lambda_j\varphi_j \circ \mathcal{T}$$

- So $\varphi_j \circ \mathcal{T}$ is an eigenfunction with eigenvalue λ_j
- This implies that λ_j has multiplicity at least two and

$$\varphi_j \circ \mathcal{T} = \sum_{\lambda_k=\lambda_j} a_{jk}\varphi_k$$

SYMMETRIES AND EIGENFUNCTIONS

- Isometries of $S^1 = [0, 2\pi) \Rightarrow \mathcal{T}_s(t) = s + t \bmod 2\pi$
- Eigenfunctions $\varphi_2(t) = \sin(t)$ and $\varphi_3(t) = \cos(t)$
- $(\varphi_2 \circ \mathcal{T}_s)(t) = \sin(s + t) = \sin(s)\cos(t) + \cos(s)\sin(t)$
- $(\varphi_3 \circ \mathcal{T}_s)(t) = \cos(s + t) = \cos(s)\cos(t) - \sin(s)\sin(t)$

$$\begin{bmatrix} \varphi_2 \circ \mathcal{T}_s \\ \varphi_3 \circ \mathcal{T}_s \end{bmatrix} = \begin{bmatrix} \cos(s) & \sin(s) \\ -\sin(s) & \cos(s) \end{bmatrix} \begin{bmatrix} \varphi_2 \\ \varphi_3 \end{bmatrix}$$

SYMMETRY GROUP REPRESENTATION

- For the n eigenfunctions with eigenvalue λ_j

$$\varphi_j \circ \mathcal{T} = \sum_{\lambda_k = \lambda_j} a_{jk} \varphi_k$$

- The matrix A with entries a_{jk} is orthogonal
- Composing isometries $\mathcal{T}_1 \circ \mathcal{T}_2$

$$\varphi_j \circ \mathcal{T}_1 \circ \mathcal{T}_2 = \sum_{\lambda_k = \lambda_j} a^1_{jk} \varphi_k \circ \mathcal{T}_2 = \sum_{\lambda_\ell = \lambda_k = \lambda_j} a^1_{jk} a^2_{k\ell} \varphi_\ell$$

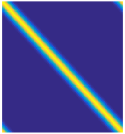
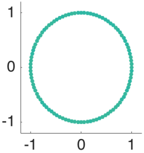
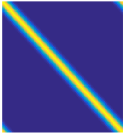
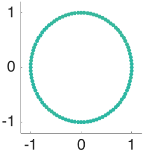
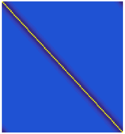
- Results in matrix multiplication
- We have a representation of the isometry group in $O(n)$!

SYMMETRY GROUP REPRESENTATION

- Isometry group has representation in orthogonal transformations of the eigenfunctions of the Laplacian
- Isometry group determines multiplicity of eigenvalues
- We can use this to search for symmetries!
- Look for repeated eigenvalues then...
- Find orthogonal transformations that preserve eigenfunctions

LAPLACIAN ON S^1, 100 POINTS

Parameterize $S^1 = \{\theta \in [0, 2\pi)\}$, Laplacian is $\Delta = -\frac{d^2}{d\theta^2}$

Kernel	Density	Normalized	Bias	Laplacian
				
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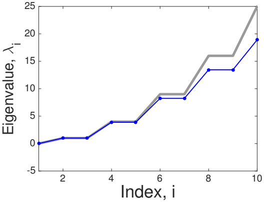

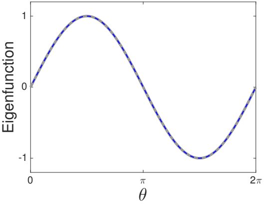

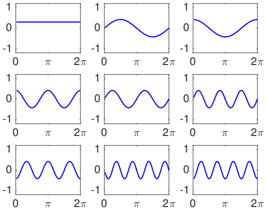

TORUS T^2, 1200 POINTS

Parameterize $T^2 = \{(\theta, \phi) \in [0, 2\pi)^2\}$

Kernel | Density | Normalized | Bias | Laplacian

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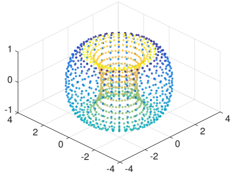
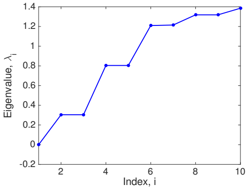
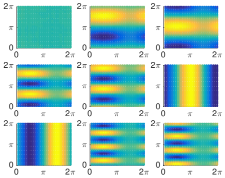
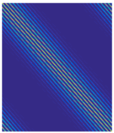
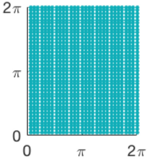
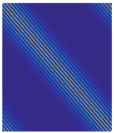
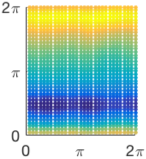
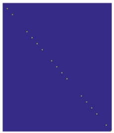


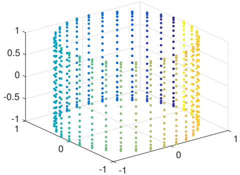


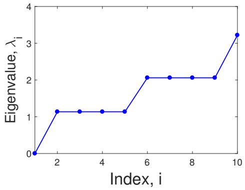


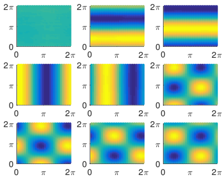
FLAT TORUS T^2, 1200 POINTS

Parameterize $T^2 = \{(\theta, \phi) \in [0, 2\pi)^2\}$

Kernel	Density	Normalized	Bias	Laplacian
				
K	$D = K1$	$\hat{K} = D^{-1}KD^{-1}$	$\hat{D} = \hat{K}1$	L

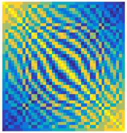
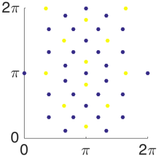
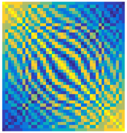
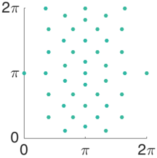
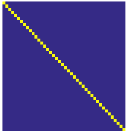


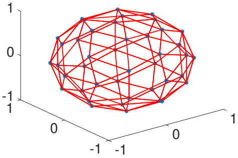


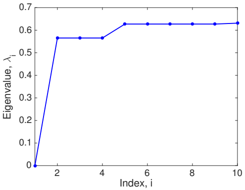


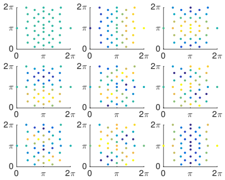
Sphere S^2, 42 points

Parameterize $S^2 = \{(\theta, \phi) \in [0, 2\pi)^2\}$

Kernel	Density	Normalized	Bias	Laplacian
				
K	$D = K1$	$\hat{K} = D^{-1}KD^{-1}$	$\hat{D} = \hat{K}1$	L



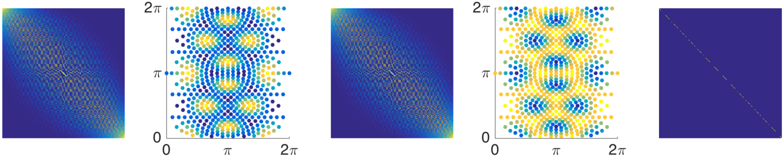




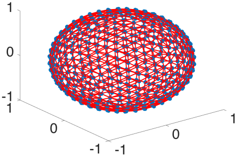
Sphere S^2, 642 points

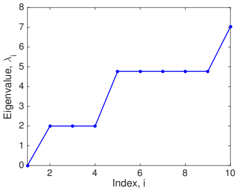
Parameterize $S^2 = \{(\theta, \phi) \in [0, 2\pi)^2\}$

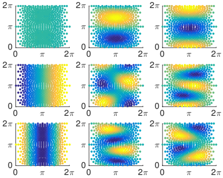
Kernel	Density	Normalized	Bias	Laplacian



K	$D = K1$	$\hat{K} = D^{-1} K D^{-1}$	$\hat{D} = \hat{K}1$	L



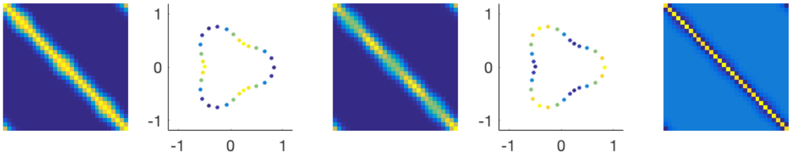




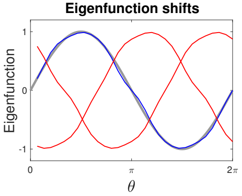
Z_3 SYMMETRY, 90 POINTS

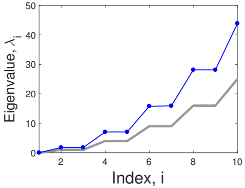
Parameterize $\{\theta \in [0, 2\pi)\}$

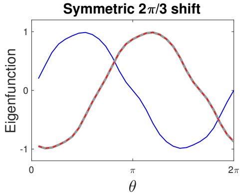
Kernel | Density | Normalized | Bias | Laplacian



K | $D = K1$ | $\hat{K} = D^{-1}KD^{-1}$ | $\hat{D} = \hat{K}1$ | L

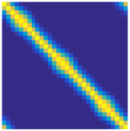
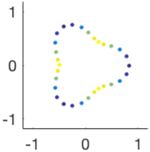
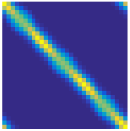
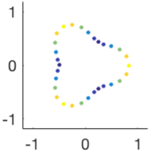
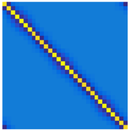


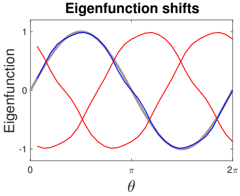


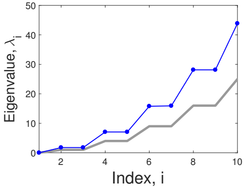


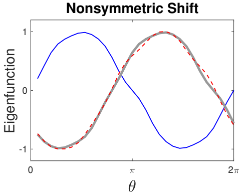
Z_3 SYMMETRY, 90 POINTS

Parameterize $\{\theta \in [0, 2\pi)\}$

Kernel	Density	Normalized	Bias	Laplacian
				
K	$D = K1$	$\hat{K} = D^{-1}KD^{-1}$	$\hat{D} = \hat{K}1$	L







SAMPLING THEORY ON MANIFOLDS

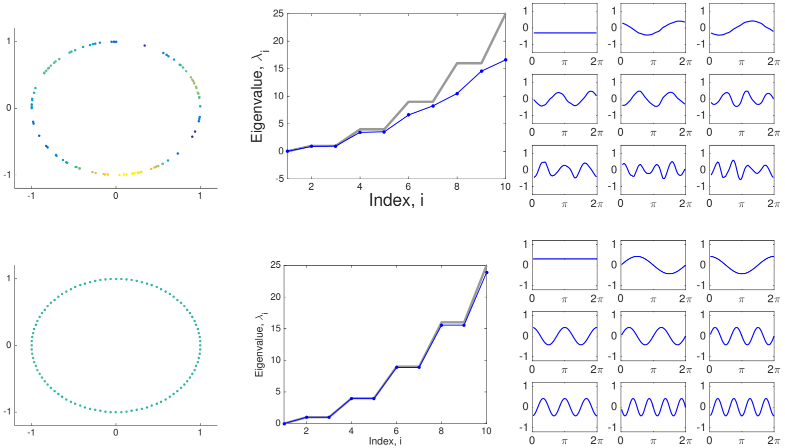
- Want to generalize Shannon's sampling theorem
- f has finite Fourier series $\Leftrightarrow$ determined by values on grid
- Assume $f(t) = a_0 + a_1 \sin(t) + a_2 \cos(t)$
- We can determine f from values on 3 points
- Best points are $\{0, 2\pi/3, 4\pi/3\}$
- Orbit of finite subgroup $Z_3 \subset O(2)$
- Finite subgroups of $O(2) \Rightarrow$ Best samples on S^1

SAMPLING THEORY ON MANIFOLDS

- Want to generalize sampling theorem to manifolds
- $\mathcal{H}_m = \text{span}\{\varphi_1, ..., \varphi_m\}$ and $K_m(x, y) = \sum_{j=1}^{m} \varphi_j(x)\varphi_j(y)$
- $f \in \mathcal{H}_m$ implies $\langle f, K_m(x, \cdot)\rangle = f(x)$ so $\mathcal{H}$ is RKHS
- Find points $x_i \in \Omega$ s.t. $\text{span}\{K_m(\cdot, x_i)\} = \mathcal{H}_m$
- **Sampling Theorem:** $f \in \mathcal{H}_m$ determined by $\vec{f}_i = f(x_i)$
- **Idea:** Sampling sets $\Leftrightarrow$ Orbits of finite subgroups of $\mathcal{T}$

SAMPLING THEORY FOR MANIFOLDS LEARNING

Good sampling sets ⇒ Fast convergence ⇒ Less data!



CONVOLUTION FUNCTION ALGEBRA

- Think of eigenfunctions φ_j as generalized Fourier basis
- In the case of S^1 recover standard Fourier basis
- On S^1 we also have multiplicative structure:

$$f * h(s) = \int_0^{2\pi} f(s-t)h(t)\,dt = \int_0^{2\pi} f(\mathcal{T}_s(t))h(t)\,dt$$

- Convolution defined in terms of translation symmetry
- Fourier transform maps convolution to multiplication
- Pontryagin duality: $\mathcal{F}(f * h) = \mathcal{F}(f)\mathcal{F}(h)$

FOURIER ANALYSIS ON MANIFOLDS

- Think of eigenfunctions φ_j as generalized Fourier basis
- Let $\mathcal{T}_{\vec{\theta}}$ be the isometry group parameterized by $\vec{\theta}$
- For a 'super-symmetric' manifold: The isometry group parameterization gives natural coordinates on the manifold
- Generalize convolution to 'super-symmetric' manifolds

$$f * h(x) = \int_{\mathcal{M}} f(\mathcal{T}_x(y))h(y)\, dy$$

- What does Pontryagin duality say?

MULTIPLICATION FUNCTION ALGEBRA

- Eigenfunctions of Δ are basis for $L^2(\mathcal{M}, g)$

$$\varphi_i \cdot \varphi_j = \sum_k c_{ijk} \varphi_k$$

- c_{ijk} are called the structure constants of the algebra
- Ex: $\varphi_2(t)\varphi_3(t) = \sin(t)\cos(t) = \sin(2t)/2 = \varphi_4(t)/2$
- Want to compute the Riemannian metric $g(v, w)$
- Fact: Any vector field can be written as $v = \sum_{ij} a_{ij} \varphi_i \nabla \varphi_j$
- So if I can compute $g(\nabla \varphi_j, \nabla \varphi_k)$ I know g

MULTIPLICATION FUNCTION ALGEBRA

- I need to compute $g(\nabla\varphi_j, \nabla\varphi_k)$, handy formula:

$$g(\nabla\varphi_j, \nabla\varphi_k) = -\frac{1}{2}\left(\varphi_i\Delta\varphi_j + \varphi_j\Delta\varphi_i - \Delta(\varphi_i\varphi_j)\right)$$

- Good thing we used eigenfunctions

$$g(\nabla\varphi_j, \nabla\varphi_k) = -\frac{1}{2}\left(\varphi_i\lambda_j\varphi_j + \varphi_j\lambda_i\varphi_i - \Delta\left(\sum_k c_{ijk}\varphi_k\right)\right)$$

- We need the structure constants!

$$g(\nabla\varphi_j, \nabla\varphi_k) = -\frac{1}{2}\sum_k c_{ijk}(\lambda_j + \lambda_i - \lambda_k)\varphi_k$$

SMOOTH EXTERIOR CALCULUS (SEC)

- Start with the smooth eigenfunctions $\Delta\varphi_i = \lambda_i\varphi_i$
- Define a frame for 1-forms: $b^{ij} = \varphi_i d\varphi_j - \varphi_j d\varphi_i$
- Define Laplace-de Rham operator on b^{ij}

$$\left\langle b^{kl}, \Delta^1(b^{ij})\right\rangle = \sum_r (c_{kir}c_{ljr} - c_{kjr}c_{lir})(\lambda_r^2 - \lambda_r(\lambda_k + \lambda_i + \lambda_l + \lambda_j)) + c_{ijr}c_{klr}(\lambda_j - \lambda_i)(\lambda_l - \lambda_k)$$

Exterior calculus is determined by function algebra

SUMMARY

- Function spaces give useful notions of convergence
- Use graph Laplacians to define discrete calculus
- Manifold symmetries represented in Laplacian eigenspace
- Graph symmetries rep. in graph Laplacian eigenspace
- Connections to convolution algebra and sampling theory
- Eigenvalues $+$ Structure constants $\Rightarrow$ Exterior Calculus