An Introduction to the Spectral Exterior Calculus

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ANALYSIS ON POINT CLOUDS

- Data lie in $\mathbb{R}^m$ for large $m \Rightarrow$ Curse-of-dimensionality
- Data may be sampled from nearly singular measures
- Geometric prior: Points lie near smooth manifold $\mathcal{M} \subset \mathbb{R}^m$
- Curse depends on the dimension $d < m$ of $\mathcal{M}$
- Goal: Learn/represent $\mathcal{M}$ with statistical error bounds

Key to Manifold Learning

- Given $f : \mathcal{M} \to \mathbb{R}$, want to estimate $\int_{\mathcal{M}} f(x)\, dx$
- Assume $\{x_i\}_{i=1}^N \subset \mathcal{M} \subset \mathbb{R}^d$ are sampled from distribution p

$$\lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^{N} f(x_i) = \mathbb{E}_{X\sim p}[f(X)] = \int_{\mathcal{M}} f(x)p(x)\, dx$$

- Step one is estimate the density p so we can compute:

$$\frac{1}{N}\sum_{i=1}^{N} \frac{f(x_i)}{p(x_i)} = \int_{\mathcal{M}} f(x)\, dx + \mathcal{O}(N^{-1/2})$$

KEY TO MANIFOLD LEARNING

- $L^2(\mathcal{M})$ inner product $\Rightarrow$ diagonal matrix $D_{ii} = \frac{1}{Np(x_i)}$

$$\vec{g}^\top D\vec{f} = \frac{1}{N}\sum_{i=1}^{N}\frac{g(x_i)f(x_i)}{p(x_i)} = \langle f, g\rangle_{L^2} + \mathcal{O}(N^{-1/2})$$

- **Quadrature Interpretation:**
  - x_i are the **nodes**
  - $w_i = \frac{1}{Np(x_i)}$ are the **weights**
- We have to estimate w_i from the data
- But any consistent quadrature rule will do! (BYOQuadrature)

Step 1: Density estimation on $\mathbb{R}^m$

- Goal: Estimate density $p(x)$ from random variables $X_i \sim p$
- Kernel density estimation on $\mathbb{R}^m$ dates from the 1950's

$$p_{h,N}(x) \equiv \frac{1}{m_0 h^m N} \sum_{i=1}^{N} K\left(\frac{||x - X_i||}{h}\right) \qquad m_0 = \int_{\mathbb{R}^m} K(||z||)\, dz$$

- Theorem: $p_{h,N}(x)$ is a consistent estimator of $p(x)$ with
- Bias: $\mathbb{E}\left[p_{h,N}(x) - p(x)\right] = \mathcal{O}(h^2)$ and
- Variance: $\mathbb{E}\left[(p_{h,N}(x) - p(x))^2\right] = \mathcal{O}\left(\frac{h^{-m}}{N} p(x)\right)$.

MANIFOLD LEARNING

- **Goal**: Represent all the information about a manifold
- Riemannian metric, g, contains all geometric information
- Laplace-Beltrami operator, Δ, is equivalent to g
- Manifold learning $\Leftrightarrow$ Estimating Laplace-Beltrami
- **Caveat:** Cannot easily answer all questions about manifold

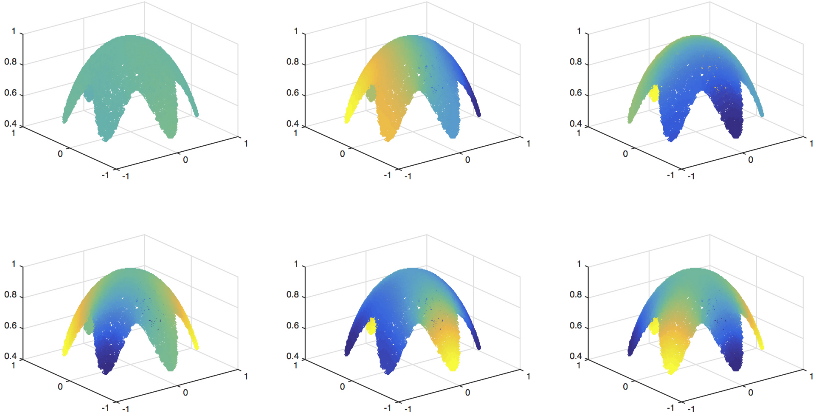
Why the Laplacian?

- **Manifold learning $\Leftrightarrow$ Estimating Laplace-Beltrami**
- Eigenfunctions $\Delta\varphi_i = \lambda_i\varphi_i$ orthonormal basis for $L^2(\mathcal{M})$
- Smoothest functions: φ_i minimizes the functional

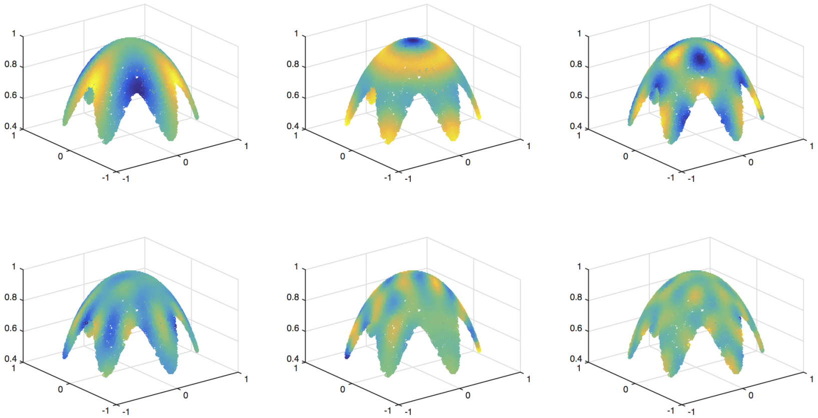
$$\lambda_i = \min_{\substack{f\perp\varphi_k \\ k=1,\dots,i-1}} \left\{ \frac{\int_{\mathcal{M}} ||\nabla f||^2 \, dV}{\int_{\mathcal{M}} |f|^2 \, dV} \right\}$$

- Eigenfunctions of Δ are custom Fourier basis
  - Smoothest orthonormal basis for $L^2(\mathcal{M})$
  - Can be used to define wavelets
  - Define the Hilbert/Sobolev spaces on $\mathcal{M}$

Harmonic Analysis on Manifolds/Data Sets



Harmonic Analysis on Manifolds/Data Sets



MATRICES AS INTEGRAL OPERATORS

- Functions are represented as vectors $\vec{f}_i = f(x_i)$
- A kernel matrix $K_{ij} = K(x_i, x_j)$ represents an operator

$$\frac{1}{N}\left(K\vec{f}\right)_i = \frac{1}{N}\sum_j K(x_i, x_j)f(x_j) \to \int_{\mathcal{M}} K(x_i, y)f(y)q(y)\,dV(y)$$

- Diagonal matrix: $D_{ii} = N^{-1}\sum_j K_{ij} = N^{-1}K\vec{1}$
- Graph Laplacian matrix: $L = \frac{1}{mh^2}\left(D^{-1}K - I\right)$
- Then $\left(L\vec{f}\right)_i = \Delta f(x_i) + \mathcal{O}(h^2)$
- This says that L is a pointwise consistent estimator of Δ

Belkin and Niyogi (2005)

DIFFUSION MAPS: ALLOWING ARBITRARY SAMPLING

- For $X_i \sim q\, dV$ on $\mathcal{M}$
- Define $K_{ij} = K\left(\frac{||x_i - x_j||}{h}\right)$ and $D_i = \sum_j K_{ij}$
- Right normalization: $\hat{K}_{ij} = K_{ij} D_j^{-1}$ and $\hat{D}_i = \sum_j \hat{K}_{ij}$
- Left normalization: $\tilde{K}_{ij} = \hat{D}_i^{-1} \hat{K}_{ij}$ and finally $L = \frac{\tilde{K} - I}{mh^2}$
- **Theorem:** L is a consistent pointwise estimator of Δ
- **Bias:** $\mathbb{E}[(L\vec{f})_i - \Delta f(x_i)] = \mathcal{O}(h^2)$
- **Variance:** $\mathbb{E}[((L\vec{f})_i - \Delta f(x_i))^2] = \mathcal{O}\left(\frac{||\nabla f(x_i)||^2 q(x_i)^{3-4d}}{N^{1/2} h^{2+d}}\right)$

Hein, Audibert, and von Luxburg (2005, 2007), Coifman and Lafon (2006)

Singer (2006), B and Harlim (2015)

WHAT ABOUT THE OTHER RIEMANNIAN STRUCTURE?

- A Riemannian manifold has an exterior calculus:
  - Calculus of tensors and differential forms
  - Built entirely from the Riemannian metric $g \Leftrightarrow \Delta$
  - Formulates the generalization of the FTC (Stokes' Thm)
  - Can construct Laplacians on k-forms, Δ_k
  - Eigenforms of Δ_k are smoothest basis for k-forms
- **Question:** Given only the eigenfunctions of the Laplacian how can we construct the rest of the exterior calculus?

WHAT ABOUT THE OTHER RIEMANNIAN STRUCTURE?

- **Good News:** Laplacian $\Leftrightarrow$ Riemannian metric

$$g(\nabla f, \nabla h) = \nabla f \cdot \nabla h = \frac{1}{2}(f\Delta h + h\Delta f - \Delta(fh))$$

- Let $v, w \in T_x\mathcal{M}$, there exists $f_1, ..., f_d$ such that $\nabla f_1, ..., \nabla f_d$ span $T_x\mathcal{M}$ and

$$g(v, w) = v \cdot w = \sum_{ij} v_i w_j \nabla f_i \cdot \nabla f_j$$

- **Bad News:** There may be no $f_1, ..., f_d$ that work for all x
- Hairy Ball Thm: Every smooth vector field on S^2 must vanish: at these points the gradients do not span $T_x\mathcal{M}$.

HOW CAN WE USE THE LAPLACIAN EIGENFUNCTIONS?

- Cannot find $\nabla f_1, ..., \nabla f_d$ basis for all $T_x\mathcal{M}$
- **Whitney:** We can find $\nabla f_1, ..., \nabla f_{2d}$ span all $T_x\mathcal{M}$
- **Thm[1]:** $\exists J$ such that $\nabla\varphi_1, ..., \nabla\varphi_J$ span all $T_x\mathcal{M}$
- Representing vector fields in a frame (overcomplete set)
  - Let $v(x) \in T_x\mathcal{M}$ be a smooth vector field
  - Then $v(x) = \sum_{j=1}^{J} c_j(x)\nabla\varphi_j(x)$ where $c_j(x)$ are smooth
  - So $c_j(x) = \sum_{i=1}^{\infty} c_{ij}\varphi_i(x)$
  - Finally $v = \sum_{i,j} c_{ij}\varphi_i\nabla\varphi_j$ (not uniquely)

[1] J. Portegies, Embeddings of Riemannian Manifolds with Heat Kernels and Eigenfunctions. (2014).

HOW CAN WE USE THE LAPLACIAN EIGENFUNCTIONS?

- **Thm (Berry & Giannakis)** Let φ_i be the eigenfunctions of the Laplacian then $\{\varphi_i \nabla \varphi_j \,:\, j = 1, ..., J, i = 1, ..., \infty\}$ is a **frame** for the L^2 space of vector fields on $\mathcal{M}$.
- A **frame** is an overcomplete spanning set commonly used in Harmonic analysis, must satisfy the frame inequalities:

$$A||v||^2 \leq \sum_{i,j} \left\langle v, \varphi_i \nabla \varphi_j \right\rangle^2 \leq B||v||^2$$

where $A, B > 0$ and $|| \cdot ||^2 = \langle \cdot, \cdot \rangle$ is the Hodge inner prod.

B & Giannakis, Spectral exterior calculus

THE SPECTRAL EXTERIOR CALCULUS (SEC)

- **Inputs:**
  - Quadrature nodes $x_i \in \mathcal{M}$ and weights w_i
  - Eigenfunctions φ_j and eigenvalues λ_j of the Laplacian
- **Outputs:**
  - Matrix representation of the 1-Laplacian as a $J^2 \times J^2$ matrix
  - Eigenforms of the 1-Laplacian $\Delta_1 \omega_j = \xi_j \omega_j$
  - Formulas for exterior derivative and many other elements of the exterior calculus

EXAMPLE: RIEMANNIAN METRIC

- Consider two 1-forms ω, ν
- Represent them in the frame (nonuniquely)

$$\omega = \sum_{ij} \omega_{ij} \phi_i d\phi_j \qquad \nu = \sum_{lk} \nu_{lk} \phi_l d\phi_k$$

- Reduce the inner product (to Hodge Grammian)

$$\langle \omega, \nu \rangle_{L^2(\Omega^1(\mathcal{M}))} = \sum_{ijlk} \omega_{ij} \nu_{lk} \left\langle \phi_i d\phi_j, \phi_l d\phi_k \right\rangle_{L^2(\Omega^1(\mathcal{M}))}$$

- Now we just need a formula on the frame elements:

$$\left\langle \phi_i d\phi_j, \phi_l d\phi_k \right\rangle_{L^2(\Omega^1(\mathcal{M}))} = \left\langle \phi_i \phi_l, d\phi_j \cdot d\phi_k \right\rangle_{L^2(\mathcal{M})}$$

EXAMPLE: RIEMANNIAN METRIC (CONTINUED)

- Apply the product rule for the Laplacian:

$$\left\langle \phi_i \phi_l, d\phi_j \cdot d\phi_k \right\rangle_{L^2(\mathcal{M})} = \frac{1}{2} \left\langle \phi_i \phi_l, \phi_j \Delta \phi_k + \phi_k \Delta \phi_j - \Delta(\phi_k \phi_j) \right\rangle_{L^2(\mathcal{M})}$$

- Since we used eigenfunctions $\Delta \phi_j = \lambda_j \phi_j$

$$= \frac{1}{2} \left\langle \phi_i \phi_l, \phi_j \lambda_k \phi_k + \phi_k \lambda_j \phi_j - \Delta(\phi_k \phi_j) \right\rangle_{L^2(\mathcal{M})}$$

- Now represent $\phi_k \phi_j = \sum_s \left\langle \phi_k \phi_j, \phi_s \right\rangle \phi_s$ and define $c_{kjs} = \left\langle \phi_k \phi_j, \phi_s \right\rangle$ then,

$$= \frac{1}{2} \left\langle \phi_i \phi_l, \phi_j \lambda_k \phi_k + \phi_k \lambda_j \phi_j - \sum_s c_{kjs} \lambda_s \phi_s \right\rangle_{L^2(\mathcal{M})}$$

EXAMPLE: RIEMANNIAN METRIC (CONTINUED)

- Finally, represent each $\phi_k\phi_j = \sum_s c_{kjs}\phi_s$

$$= \frac{1}{2}\sum_s (\lambda_k + \lambda_j - \lambda_s) c_{kjs} \langle \phi_i\phi_l, \phi_s \rangle$$

- Note the triple produce $c_{ils} = \langle \phi_i\phi_l, \phi_s \rangle$ appears again,

$$G_{ijkl} \equiv \left\langle \phi_i d\phi_j, \phi_l d\phi_k \right\rangle_{L^2(\Omega^1(\mathcal{M}))} = \frac{1}{2}\sum_s (\lambda_k + \lambda_j - \lambda_s) c_{kjs} c_{ils}$$

- Now we can apply to any 1-forms,

$$\langle \omega, \nu \rangle_{L^2(\Omega^1(\mathcal{M}))} = \sum_{ijlk} \omega_{ij} \nu_{lk} G_{ijkl}$$

EXAMPLE: RIEMANNIAN METRIC (RECAP)

- Now we can apply to any 1-forms,

$$\langle \omega, \nu \rangle_{L^2(\Omega^1(\mathcal{M}))} = \sum_{ijlk} \omega_{ij} \nu_{lk} G_{ijkl}$$

- To build G_{ijkl} we need:
  - Eigenfunctions and eigenvalues of Δ to use product rule
  - The symmetric triple product $c_{ijk} = \langle \phi_i \phi_j, \phi_k \rangle$
  - We can compute c_{ijk} from our quadrature rule

- While far from obvious, these simple elements can build entire exterior calclulus

A CALCULUS NEEDS FORMULAS!

Object	Symbolic	Spectral
Function	f	$\hat{f}_k = \langle \phi_k, f \rangle_{L^2}$
Laplacian	Δf	$\langle \phi_k, \Delta f \rangle_{L^2} = \lambda_k \hat{f}_k$
L^2 Inner Product	$\langle f, h \rangle_{L^2}$	$\sum_i \hat{f}_i^* \hat{h}_i$
Dirichlet Energy	$\langle f, \Delta f \rangle_{L^2}$	$\sum_i \lambda_i \lvert \hat{f}_i \rvert^2$
Multiplication	$\phi_i \phi_j$	$c_{ijk} = \left\langle \phi_i \phi_j, \phi_k \right\rangle_{L^2}$
Function Product	fh	$\sum_{ij} c_{kij} \hat{f}_i \hat{h}_j$
Riemannian Metric	$\nabla \phi_i \cdot \nabla \phi_j$	$g_{kij} \equiv \left\langle \nabla \phi_i \cdot \nabla \phi_j, \phi_k \right\rangle_{L^2} = \frac{1}{2}(\lambda_i + \lambda_j - \lambda_k) c_{kij}$
Gradient Field	$\nabla f(h) = \nabla f^* \cdot \nabla h$	$\langle \phi_k, \nabla f(h) \rangle_{L^2} = \sum_{ij} g_{kij} \hat{f}_i \hat{h}_j$
Exterior Derivative	$df(\nabla h) = df^* \cdot dh$	$\sum_{ij} g_{kij} \hat{f}_i \hat{h}_j$
Vector Field (basis)	$v(f) = v^* \cdot \nabla f$	$\sum_j v_{ij} \hat{f}_j$
Divergence	$\mathrm{div} v$	$\langle \phi_i, \mathrm{div} v \rangle_{L^2} = -v_{0i}$
Frame Elements	$b_{ij}(\phi_l) = \phi_i \nabla \phi_j (\phi_l)$	$G_{ijkl} \equiv \left\langle b_{ij}(\phi_l), \phi_k \right\rangle_{L^2} = \sum_m c_{mik} g_{mjl}$
Vector Field (frame)	$v(f) = \sum_{ij} v^{ij} b_{ij}(f)$	$\langle \phi_k, v(f) \rangle_{L^2} = \sum_{ijl} G_{ijkl} v^{ij} \hat{f}_l$
Frame Elements	$b^{ij}(v) = b^i \, db^j(v)$	$\left\langle \phi_k, b^{ij}(v) \right\rangle_{L^2} = \sum_{nlm} c_{kmi} G_{nlmj} v^{nl}$
1-Forms (frame)	$\omega = \sum_{ij} \omega_{ij} b^{ij}$	$\langle \phi_k, \omega(v) \rangle_{L^2} = \sum_{ij} \omega_{ij} \left\langle \phi_k, b^{ij}(v) \right\rangle_{L^2}$

Operator	Tensor	Symmetries
Quadruple Product	$c^0_{ijkl} = \left\langle \phi_i \phi_j, \phi_k \phi_l \right\rangle_{L^2} = \sum_s c_{ijs} c_{skl}$	Fully symmetric
Product Energy	$c^p_{ijkl} = \left\langle \Delta^p(\phi_i \phi_j), \phi_k \phi_l \right\rangle_{L^2} = \sum_s \lambda^p_s c_{ijs} c_{skl}$	(1,2), (3,4), (1,3), (2,4)
Hodge Grammian	$G_{ijkl} = \left\langle b^{ij}, b^{kl} \right\rangle_{L^2_1} = \frac{1}{2}\left[(\lambda_j + \lambda_l) c^0_{ijkl} - c^1_{ijkl}\right]$	(1,3), (2,4)
Antisymmetric	$\hat{G}_{ijkl} = \langle \hat{b}^{ij}, \hat{b}^{kl} \rangle_{L^2_1} = G_{ijkl} + G_{jilk} - G_{jikl} - G_{ijlk}$	(1,3), (2,4)
Dirichlet Energy $E_{ijkl} = \left\langle b^{ij}, \Delta_1(b^{kl}) \right\rangle_{L^2_1}$	$E_{ijkl} = \frac{1}{4}\left[(\lambda_i + \lambda_j + \lambda_k + \lambda_l)(c^1_{iljk} - c^1_{ikjl}) + (\lambda_j + \lambda_l - \lambda_i - \lambda_k) c^1_{ijkl} + (c^2_{ijkl} + c^2_{ikjl} - c^2_{iljk})\right]$	(1,3), (2,4)
Antisymmetric	$\hat{E}_{ijkl} = \langle \hat{b}^{ij}, \Delta_1 \hat{b}^{kl} \rangle_{L^2_1} = (\lambda_i + \lambda_j + \lambda_k + \lambda_l)(c^1_{iljk} - c^1_{ikjl}) + (c^2_{ikjl} - c^2_{iljk})$	(1,3), (2,4)
Sobolev H^1 Grammian	$G^1_{ijkl} = E_{ijkl} + G_{ijkl}, \ \hat{G}^1_{ijkl} = \hat{E}_{ijkl} + \hat{G}_{ijkl}$	(1,3), (2,4)

Object	Symbolic	Spectral
Multiple Product	$c^0_I = \left\langle b^{i_0} \cdots b^{i_k}, 1 \right\rangle_H$	$c^0_I = \sum_s c_{i_0 i_1 s} c^0_{s i_2 \cdots i_k}$
Tensor	$H^{\tilde{I}\tilde{J}} = (db^{i_1} \cdot db^{j_1}) \cdots (db^{i_k} \cdot db^{j_k})$	$\hat{H}^{\tilde{I}\tilde{J}}_l \equiv \langle H^{\tilde{I}\tilde{J}}, b^l \rangle_H$
Evaluation	$= \nabla b^{i_1} \otimes \cdots \otimes \nabla b^{i_k}(b^{j_1}, \ldots, b^{j_k})$	$= \sum_{n=1}^{k^2} \prod_{s,r=1}^{k} g_{i_s j_r m_n} c_{l m_1 \cdots m_{k^2}}$
Tensor Product	$b_J = b^{j_0} \nabla b^{j_1} \otimes \cdots \otimes \nabla b^{j_k}$	$\left\langle b_J(b^{i_1}, \ldots, b^{i_k}), b^l \right\rangle = \sum_s \hat{H}^{\tilde{J}\tilde{I}}_s c_{s j_0 l}$
Frame Elements	$b^I = b^{i_0} db^{i_1} \wedge \cdots \wedge db^{i_k}$	$\left\langle b^I(b_J), b^l \right\rangle_H = \left\langle b^I \cdot b^J, b^l \right\rangle_H$
Riemannian Metric	$b^I \cdot b^J = b^{i_0} b^{j_0} \det([db^{i_q} \cdot db^{j_n}])$	$\left\langle b^I \cdot b^J, b_l \right\rangle_H = \sum_s \sum_{\sigma \in S_k} \mathrm{sgn}(\sigma) c_{s i_0 j_0 l} \hat{H}^{\tilde{I}\sigma(\tilde{J})}_s$
Hodge Grammian	$G_{IJ} = \left\langle b^I, b^J \right\rangle_{H_k} = \left\langle b^I \cdot b^J, 1 \right\rangle_H$	$\sum_s \sum_{\sigma \in S_n} \mathrm{sgn}(\sigma) c_{s i_0 j_0} \hat{H}^{\tilde{I}\sigma(\tilde{J})}_s$
d-Energy	$E^d_{IJ} = \left\langle db^I, db^J \right\rangle_{H_{k+1}}$	$\left\langle db^I \cdot db^J, 1 \right\rangle_{H_{k+1}} = \hat{H}^{IJ}_0$

BACK TO BASIS

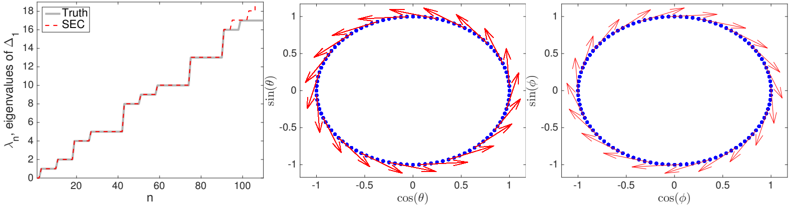
- We need the frame representation to build the 1-Laplacian

$$\Delta_1 = d\delta + \delta d$$

- Eigenfields of $\Delta_1 \Rightarrow$ smoothest basis for vector fields
- Can use to smooth vector fields and represent operators

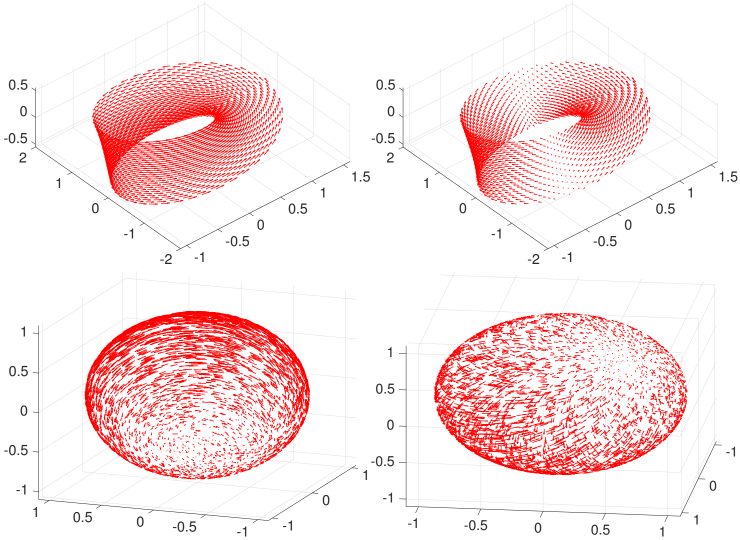
NUMERICAL VERIFICATION ON FLAT TORUS

Captures the true spectrum of the Hodge Laplacian.

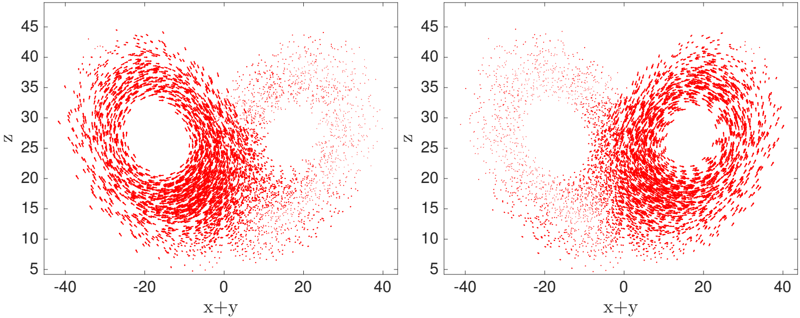


Harmonic forms correspond to unique homology classes.

SMOOTHEST VECTOR FIELDS ON THE MANIFOLD



SEC is applicable to any data set



Matlab Code: http://math.gmu.edu/~berry/

WHY THE SEC?

- Other approaches represent 1-forms as edge weights
- 5000 nodes means at least 20000 edges
- So the 1-Laplacian would be a 20000 $\times$ 20000 matrix!
- We often only want to represent smooth forms
- These will be well represented using the frame $\{\phi_i d\phi_j\}$
- We can choose how many frame elements to use, independent of the number of nodes
- Fewer elements just means more implicit smoothing/regularization

Matlab Code: http://math.gmu.edu/˜berry/