Manifold Learning and Grid-Free Methods with the Spectral Exterior Calculus (SEC)

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FFT
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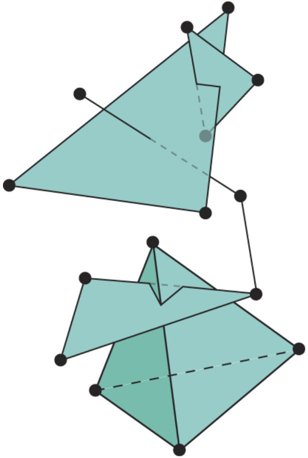
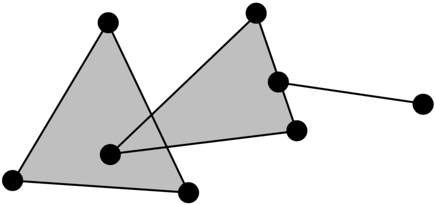
DATA ESSENTIALS

- Most data comes with: similarity/dissimilarity
- Similarity/dissimilarity $\Rightarrow$ Graph structure
- Graph structure $\Rightarrow$ Graph Laplacian
- +Diffusion Maps $\Rightarrow$ Manifold Laplacian
- +SEC $\Rightarrow$ All the geometry

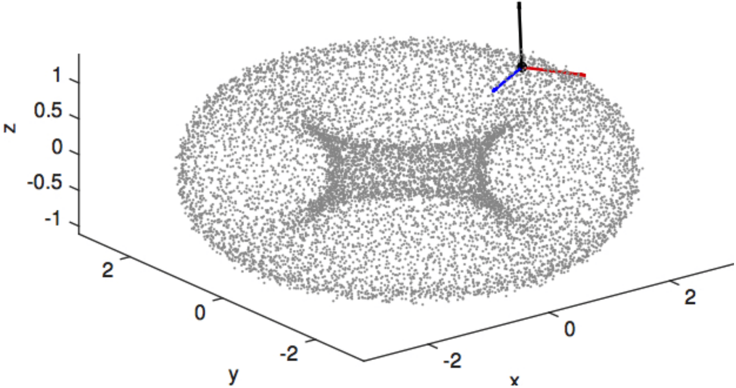
SIMPLICIAL COMPLEXES ARE COMPLEX





HOW NOT TO LEARN A MANIFOLD

Triangulate this:



Graph ⇔ Laplacian ⇔ Manifold

- **Graph Laplacian ⇔ Encodes Entire Graph**
- Smoothest functions: $(D - A)\vec{\phi}_\ell = \lambda_\ell D\vec{\phi}_\ell$ minimizes

$$\lambda_\ell = \min_{\substack{\vec{v} \perp \vec{\phi}_k \\ k=1,\ldots,\ell-1}} \left\{ \frac{\frac{1}{2}\sum_{ij} A_{ij}(\vec{v}_i - \vec{v}_j)^2}{\sum_i D_{ii}\vec{v}_i^2} \right\}$$

- Harmonic analysis ⇒ Convolutions / wavelets on graphs

GRAPH ⇔ LAPLACIAN ⇔ MANIFOLD

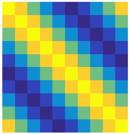
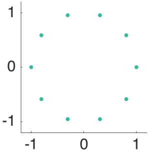
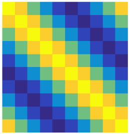
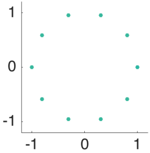
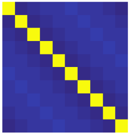
- **Laplace-Beltrami ⇔ Encodes Entire Manifold**
- Eigenfunctions $\Delta\varphi_\ell = \lambda_\ell \varphi_\ell$ orthonormal basis for $L^2(\mathcal{M})$
- Smoothest functions: φ_ℓ minimizes the functional

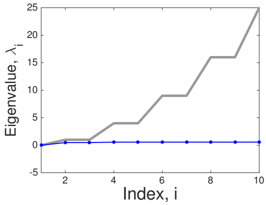
$$\lambda_\ell = \min_{\substack{f \perp \varphi_k \\ k=1,\ldots,\ell-1}} \left\{ \frac{\int_{\mathcal{M}} ||\nabla f||^2 \, dV}{\int_{\mathcal{M}} |f|^2 \, dV} \right\}$$

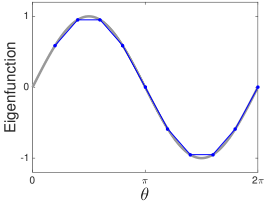
- Harmonic analysis ⇒ Convolutions / wavelets on manifolds

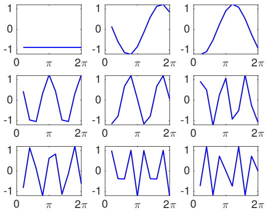
LAPLACIAN ON S^1, 10 POINTS

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

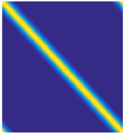
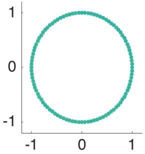
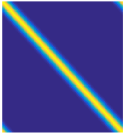
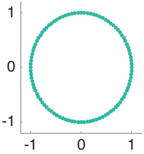
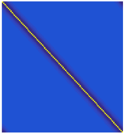


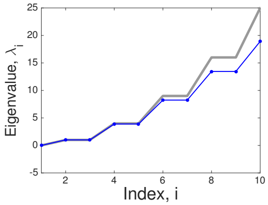


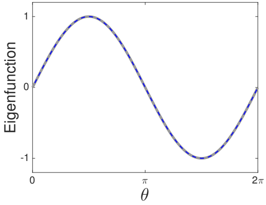


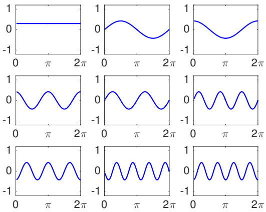
LAPLACIAN ON S^1, 100 POINTS

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

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



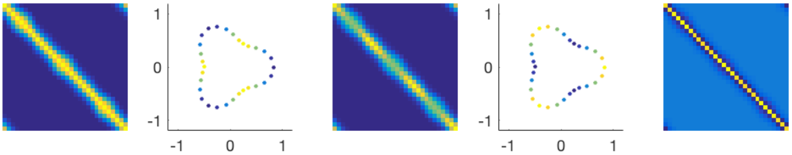




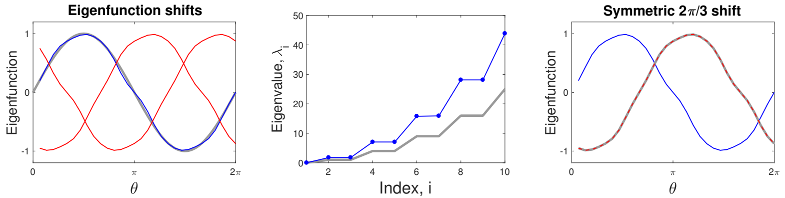
Z_3 SYMMETRY, 90 POINTS

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

Kernel Density Normalized Bias Laplacian



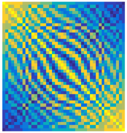
K $D = K1$ $\hat{K} = D^{-1}KD^{-1}$ $\hat{D} = \hat{K}1$ L



SPHERE S^2, 42 POINTS

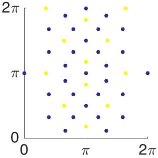
Parameterize $S^2 = \{(\theta, \phi) \in [0, 2\pi)^2\}$

Kernel



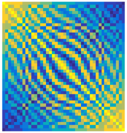
K

Density



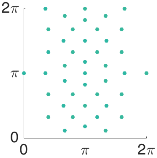
$D = K1$

Normalized



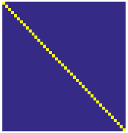
$\hat{K} = D^{-1}KD^{-1}$

Bias

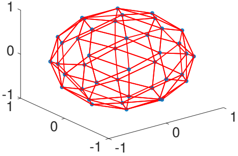


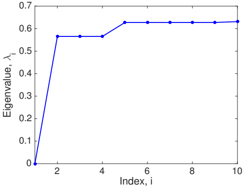
$\hat{D} = \hat{K}1$

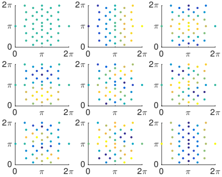
Laplacian



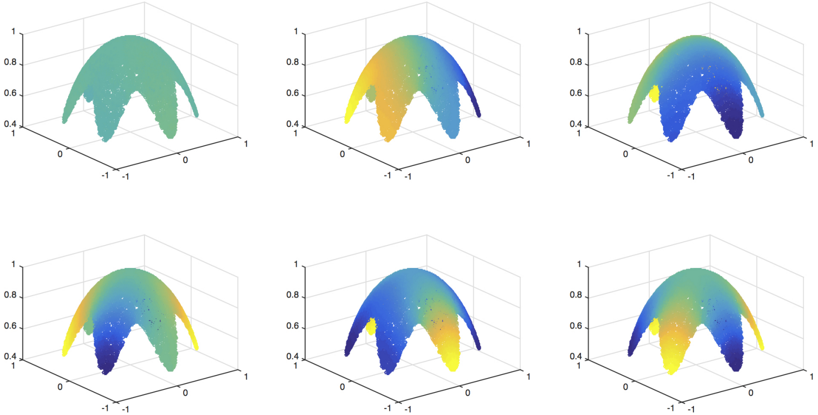
L



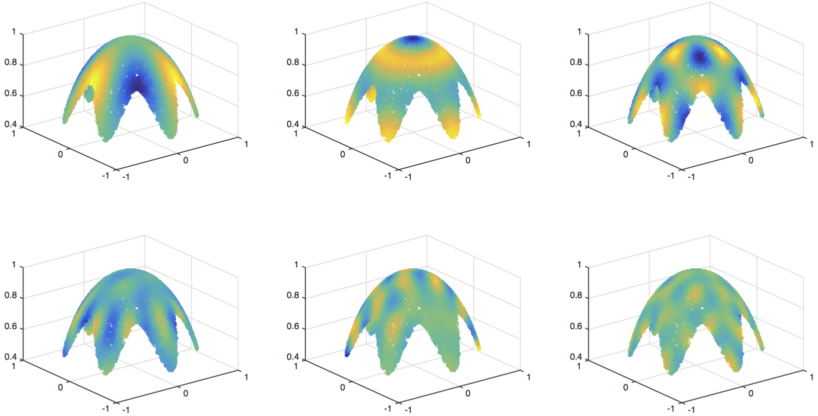




Harmonic Analysis on Manifolds/Graphs



HARMONIC ANALYSIS ON MANIFOLDS/GRAPHS



WHAT ABOUT THE OTHER RIEMANNIAN STRUCTURE?

- A Riemannian manifold has an exterior calculus:
  - Calculus of tensor fields and differential forms
  - Built entirely from the Riemannian metric $g \Leftrightarrow \Delta$
  - Geometry meets harmonic analysis:
    - Formulates the generalization of the FTC (Stokes' Thm)
    - Nonlinear observability/controllability (Lie deriv.)
    - Hodge/Helmholtz decomp., etc.
- **Graph/Manifold** $\Leftrightarrow$ **Laplacian** $\Leftrightarrow \{(\phi_i, \lambda_i)\} \Leftrightarrow$ **SEC**

Graph/Manifold $\Leftrightarrow$ Laplacian $\Leftrightarrow$ $\{(\phi_i, \lambda_i)\}$ $\Leftrightarrow$ SEC

- Laplacian $\Leftrightarrow$ Pointwise dot product on gradient fields

$$\Delta(fh) = f\Delta h + h\Delta f - 2\nabla f \cdot \nabla h$$

- So given any gradient fields $\nabla f, \nabla h$ we can define,

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

Graph/Manifold $\Leftrightarrow$ Laplacian $\Leftrightarrow \{(\phi_i, \lambda_i)\} \Leftrightarrow$ SEC

- For eigenfunctions of Δ,

$$\begin{aligned}\nabla\phi_i \cdot \nabla\phi_j &\equiv \frac{1}{2}(\phi_i\Delta\phi_j + \phi_j\Delta\phi_i - \Delta(\phi_i\phi_j)) \\ &= \frac{1}{2}((\lambda_i + \lambda_j)\phi_i\phi_j - \Delta(\phi_i\phi_j))\end{aligned}$$

- So we need to understand/encode the product algebra on smooth functions

Graph/Manifold $\Leftrightarrow$ Laplacian $\Leftrightarrow$ $\{(\phi_i, \lambda_i)\}$ $\Leftrightarrow$ SEC

- Any smooth $f = \sum_i \hat{f}_i \phi_i$, so

$$fh = \sum_{ij} \hat{f}_i \hat{h}_j \phi_i \phi_j$$

- $\phi_i \phi_j$ is smooth, so $\phi_i \phi_j = \sum_k c_{ijk} \phi_k$
- Structure constants $c_{ijk} = \langle \phi_i \phi_j, \phi_k \rangle$ encode the algebra

Graph/Manifold $\Leftrightarrow$ Laplacian $\Leftrightarrow$ $\{(\phi_i, \lambda_i)\}$ $\Leftrightarrow$ SEC

- Structure constants $c_{ijk} = \langle \phi_i \phi_j, \phi_k \rangle$ encode the algebra

$$
\begin{aligned}
\nabla \phi_i \cdot \nabla \phi_j &= \frac{1}{2}((\lambda_i + \lambda_j)\phi_i\phi_j - \Delta(\phi_i\phi_j)) \\
&= \frac{1}{2}\left((\lambda_i + \lambda_j)\sum_k c_{ijk}\phi_k - \Delta\left(\sum_k c_{ijk}\phi_k\right)\right) \\
&= \frac{1}{2}\sum_k c_{ijk}(\lambda_i + \lambda_j - \lambda_k)\phi_k
\end{aligned}
$$

- Fourier coeffs: $\langle \nabla \phi_i \cdot \nabla \phi_j, \phi_k \rangle = \frac{1}{2}\sum_k c_{ijk}(\lambda_i + \lambda_j - \lambda_k)$

What about non-gradient fields?

- 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

$$v \cdot w = \sum_{ij} v_i w_j \nabla f_i \cdot \nabla f_j$$

- **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 $T_x\mathcal{M}$.

What about non-gradient fields?

- 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 $\nabla \phi_1, ..., \nabla \phi_J$ span all $T_x\mathcal{M}$
- Overcomplete $\Rightarrow$ We need a frame!

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

BUILDING A FRAME FOR VECTOR FIELDS

- 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)

Building a frame

- **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:**
  - Eigenfunctions φ_j and eigenvalues λ_j of the Laplacian
- **Outputs:**
  - Matrix representation of the 1-Laplacian
  - Eigenforms of the 1-Laplacian $\Delta_1 \omega_j = \xi_j \omega_j$
  - Formulas for many elements of the exterior calculus

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	$c^p_{ijkl} = \left\langle \Delta^p(\phi_i\phi_j), \phi_k\phi_l \right\rangle_{L^2} = \sum_s \lambda_s^p c_{ijs}c_{skl}$	(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	$G^1_{ijkl} = E_{ijkl} + G_{ijkl}, \quad \hat{G}^1_{ijkl} = \hat{E}_{ijkl} + \hat{G}_{ijkl}$	(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	$H^{\tilde{I}\tilde{J}} = (db^{i_1} \cdot db^{j_1}) \cdots (db^{i_k} \cdot db^{j_k})$	$\hat{H}^{\tilde{I}\tilde{J}}_I \equiv \langle H^{\tilde{I}\tilde{J}}, b^I \rangle_H$
Evaluation	$= \nabla b^{i_1} \otimes \cdots \otimes \nabla b^{i_k}(b^{j_1}, \ldots, b^{j_k})$	$= \sum_{n=1}^{k^2} \prod_{s,r=1}^{k} g_{i_s j_r m_n} c_{I m_1 \cdots m_{k^2}}$
Tensor Product	$b_J = b^{j_0} \nabla b^{j_1} \otimes \cdots \otimes \nabla b^{j_k}$	$\left\langle b_J(b^{i_1}, \ldots, b^{i_k}), b^I \right\rangle = \sum_s \hat{H}^{\tilde{J}\tilde{I}}_s c_{s j_0 I}$
Frame Elements	$b^I = b^{i_0} db^{i_1} \wedge \cdots \wedge db^{i_k}$	$\left\langle b^I(b_J), b^I \right\rangle_H = \left\langle b^I \cdot b^J, b^I \right\rangle_H$
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

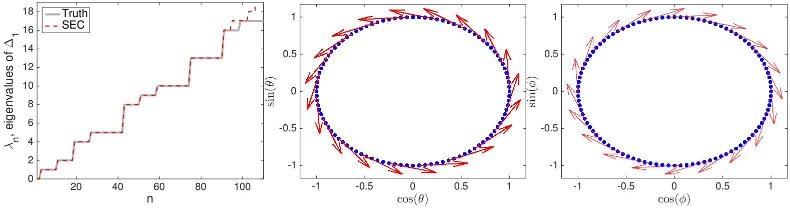
$$\Delta_1 = d\delta + \delta d$$

$$E_{ij,kl} = \langle \phi_i d\phi_j, \Delta_1(\phi_k d\phi_l) \rangle$$

- Eigenfields of $\Delta_1 \Rightarrow$ Harmonic analysis on vector fields
- Can use to smooth vector fields and represent operators

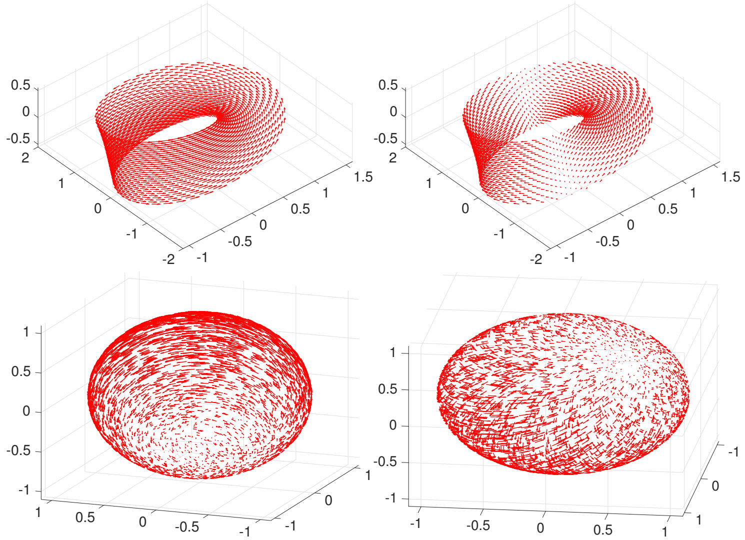
Numerical Verification on Flat Torus

Captures the true spectrum of the Hodge Laplacian.

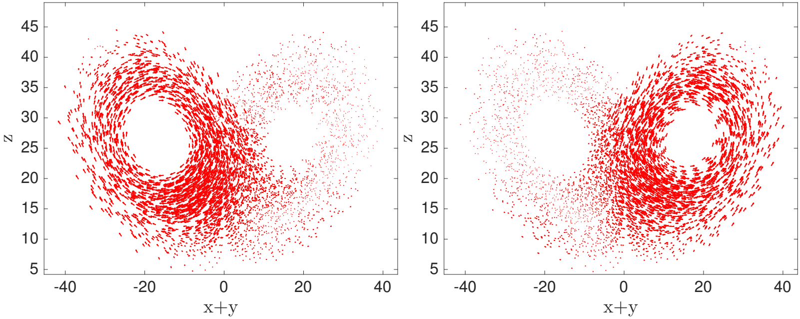


Harmonic forms correspond to unique homology classes.

Smoothest vector fields on the manifold



SEC IS APPLICABLE TO ANY GRAPH/DATA SET



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

SEC vs. DEC/FEEC

- **Data Structure:**
  - DEC/FEEC require a simplicial complex
  - SEC only requires a graph
- **Complexity:**
  - DEC/FEEC represent forms as edge weights
    - N nodes $\Rightarrow$ order-Nk edges
    - So the 1-Laplacian would be a $Nk \times Nk$ matrix
  - SEC decouples complexity from N
    - Depends on # of eigenfunctions $\Rightarrow$ resolution
- **Consistency/Topology:**
  - DEC/FEEC have strong topological consistency
  - SEC currently only has asymptotic topological consistency

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