Spectral Exterior Calculus for Dynamics

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ANALYZING DYNAMICAL SYSTEMS FROM DATA

- What is manifold learning? $\Rightarrow$ Custom Fourier Basis
- **Spectral Exterior Calculus (SEC)**
  - Represents everything about the manifold in the basis
  - Generalizes exterior calculus to graphs/point clouds
- Analyzing dynamics: Decomposing vector fields w/ SEC

WHAT IS MANIFOLD LEARNING?

- Geometric prior: Data lie on/near manifold $\mathcal{M} \subset \mathbb{R}^m$
- **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

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

- Eigenfunctions of Δ are a generalized Fourier basis

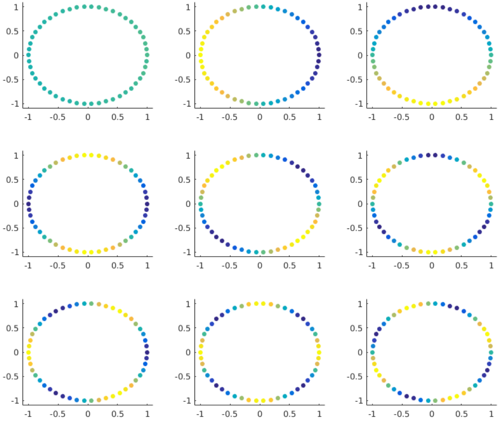
SO HOW DO WE FIND THE LAPLACIAN FROM DATA?

- Data set $\Rightarrow$ *weighted graph*
- Normalized graph Laplacian: $\mathbf{L} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{K}$
- **Theorem:** In an appropriate limit of large data we have

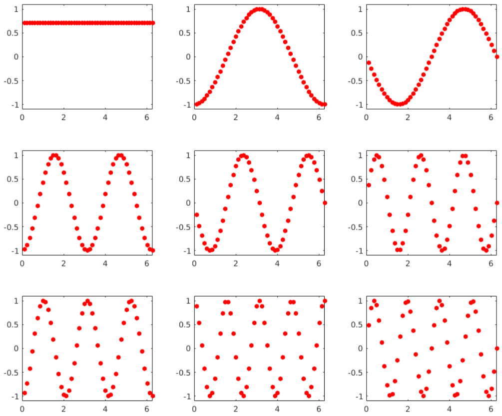
$$L \to \Delta$$

- Eigenvectors $\vec{\phi}$ of L converge to eigenfunctions φ of Δ

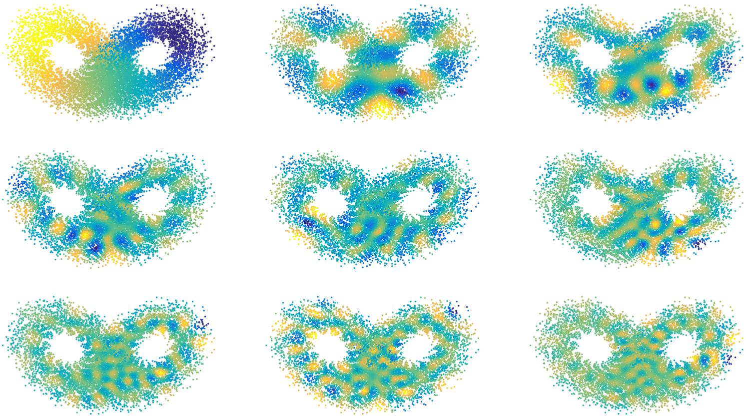
EXAMPLE S^1: EIGENVECTORS ON DATA



EXAMPLE S^1: EIGENVECTORS VS. θ



Harmonic Analysis on Manifolds/Data Sets



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 ⇔ 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.

T. Berry & D. Giannakis, Spectral exterior calculus. (Preprint available on arXiv)

THE SPECTRAL EXTERIOR CALCULUS (SEC)

- We extend Thm to frames for Sobolev spaces of tensors
- SEC formulates the entire exterior calculus in these frames
- Key accomplishment: Representation of the 1-Laplacian

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

- Key challenge: Frame representations are not unique, requires Sobolev regularizations for numerical stability

T. Berry & D. Giannakis, Spectral exterior calculus. (Preprint available on arXiv)

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	$G^1_{ijkl} = E_{ijkl} + G_{ijkl}, \quad \hat{G}^1_{ijkl} = \hat{E}_{ijkl} + \hat{G}_{ijkl}$	(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 Evaluation	$H^{\tilde{I}\tilde{J}} = (db^{i_1} \cdot db^{j_1}) \cdots (db^{i_k} \cdot db^{j_k}) = \nabla b^{i_1} \otimes \cdots \otimes \nabla b^{i_k}(b^{j_1}, \ldots, b^{j_k})$	$\hat{H}^{\tilde{I}\tilde{J}}_l \equiv \langle H^{\tilde{I}\tilde{J}}, b^l \rangle_H = \sum_{n=1}^{k^2} \prod_{s,r=1}^{k} g_{i_s j_r m_n} c_{l m_1 \cdots m_{k^2}}$
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	$b^I \cdot b^J = b^{i_0} b^{j_0} \det([db^{i_q} \cdot db^{j_n}])$	$\left\langle b^I \cdot b^J, b_l \right\rangle_H = \sum_s \sum_{\sigma \in S_k} \operatorname{sgn}(\sigma) c_{s i_0 j_0 l} \hat{H}^{\tilde{I}\sigma(\tilde{J})}_s$
Hodge Grammian	$G_{IJ} = \left\langle b^I, b^J \right\rangle_{H_k} = \left\langle b^I \cdot b^J, 1 \right\rangle_H$	$\sum_s \sum_{\sigma \in S_n} \operatorname{sgn}(\sigma) c_{s i_0 j_0} \hat{H}^{\tilde{I}\sigma(\tilde{J})}_s$
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

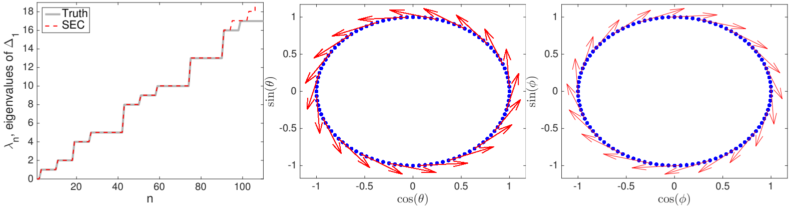
- We need the frame representation to build the 1-Laplacian

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

- Once we have Δ_1, the eigenfields form the smoothest possible basis for vector fields
- Can use to smooth vector fields and represent operators

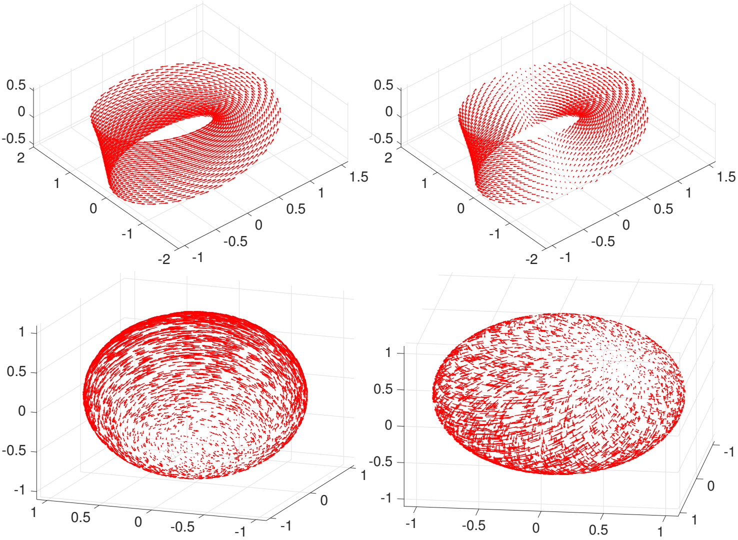
Numerical Verification on Flat Torus

Captures the true spectrum of the Hodge Laplacian.

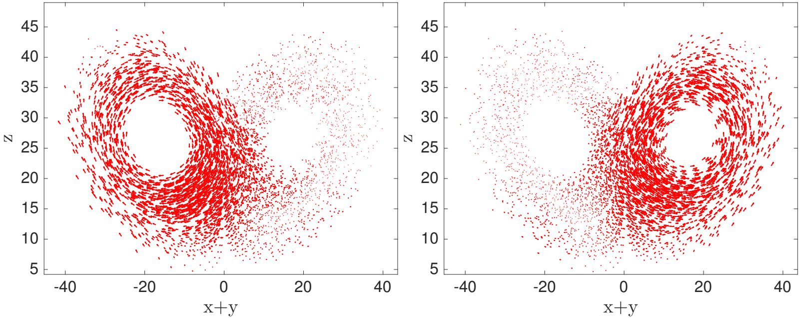


Harmonic forms correspond to unique homology classes.

SMOOTHEST VECTOR FIELDS ON THE MANIFOLD



SEC IS APPLICABLE TO ANY DATA SET



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

Applying the SEC to Dynamical Systems

- Smooth/Denoise vector fields using SEC basis
- Compute Lyapunov vector fields in the SEC basis
- Next Step: Hodge decomposition

$$v = \nabla U + \delta A + v^{\perp}$$

- U is a potential, A is a tensor field, and $\Delta_1 v^{\perp} = 0$

DECOMPOSING SDE COMPONENTS

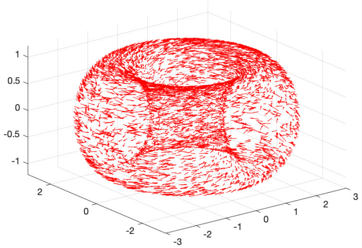
- Given a realization of an SDE on a manifold:

$$dx = f(x)\,dt + B(x)\,dW_t$$

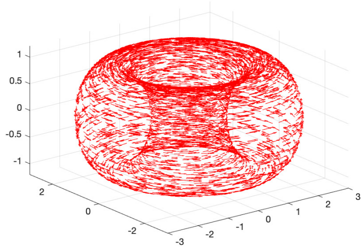
- Want to extract the deterministic component, $f(x)$
- Finite differences $x(t+\tau) - x(t) \approx f(x(t))$ but noisy
- Can smooth component functions using DM basis
- Better to smooth with SEC eigenvectorfields

Decomposing SDE Components

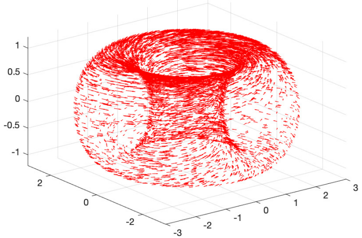
Finite Difference Est.



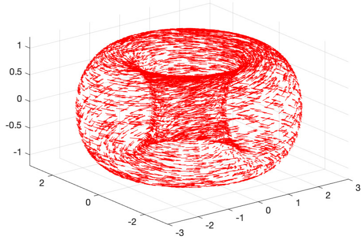
True Vector Field



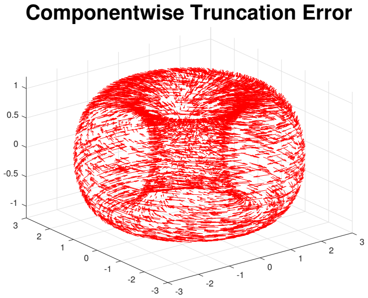
Componentwise Truncation

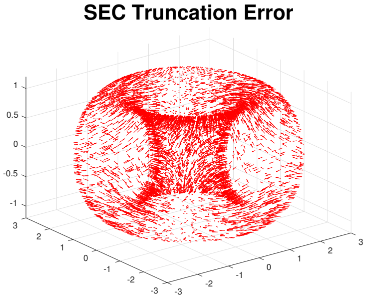


SEC Truncation



DECOMPOSING SDE COMPONENTS





Finding Lyapunov Vector Fields

- Given a vector field f, covariant Lyapunov vector fields:

$$Df(x_t)v_{x_t} = v_{x_{t+1}} = S(v_{x_t})$$

- Represent *Df* and *S* in the basis of eigenvectorfields

$$[Df]_{ij} = \left\langle v_i, Dfv_j \right\rangle \qquad [S]_{ij} = \left\langle v_i, Sv_j \right\rangle$$

- Compute the generalized eigenvectors $[Df]\vec{c} = \lambda[S]\vec{c}$
- Reconstruct Lyapunov fields $v = \sum_i \vec{c}_i v_i$

Problem: Lyapunov Vector Fields Not Smooth