Manifold Learning, Explanations and Eigenflows

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Geometry and Statistics in Data Sciences
Institut Henri Poincaré
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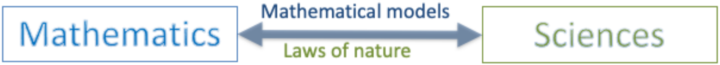
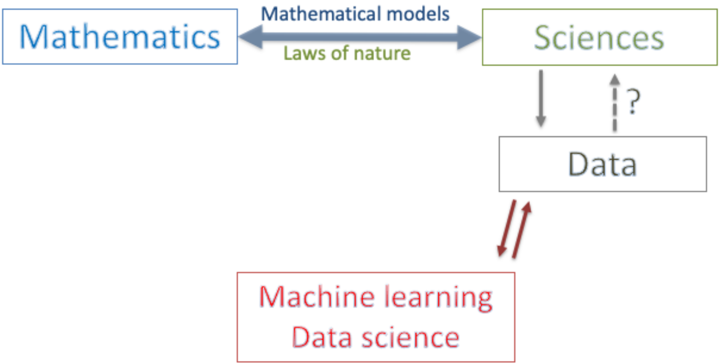

Mathematics
Mathematical models
Laws of nature
Sciences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Sciences
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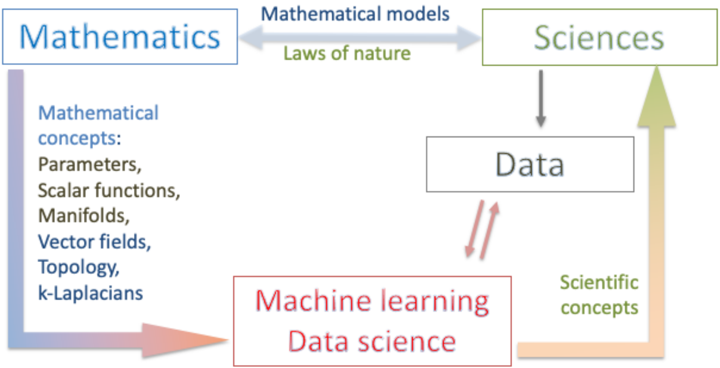
Data
Machine learning
Data science


Mathematics
Mathematical models
Laws of nature
Sciences
Mathematical concepts:
Parameters,
Scalar functions,
Manifolds,
Vector fields,
Topology,
k-Laplacians
Data
Machine learning
Data science
Scientific concepts

Outline

Manifold coordinates with Scientific meaning

Machine Learning 1-Laplacians, topology, vector fields

- 1-Laplacian $\Delta_1(\mathcal{M})$ estimation from samples
- Analysis of vector fields – Helmholtz-Hodge decomposition
- Harmonic Embedding Spectral Decomposition Algorithm
- Spectral Shortest Homologous Loop Detection

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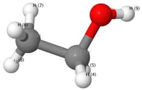
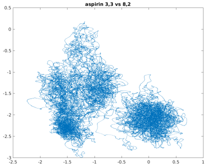
Motivation – understanding data from a Molecular Dynamics simulation

ethanol



original
data



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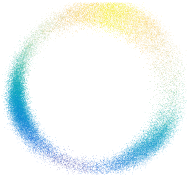

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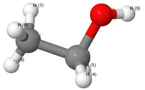

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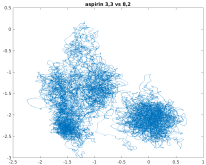
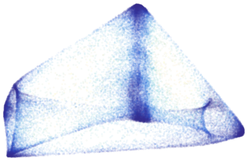


after manifold learning



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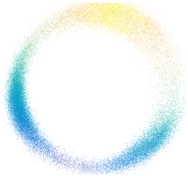

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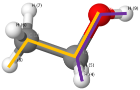

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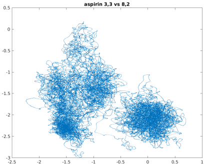
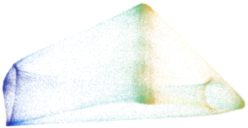


torsion 1



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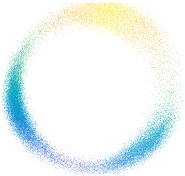
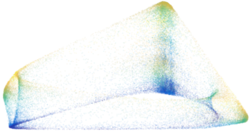


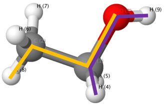
torsion 2



- 2 rotation angles (torsions) describe this manifold
- Can we discover these features automatically? Can we select these angles from a larger set of features with physical meaning?

scientific language (torsions)

data driven coordinates (from DiffMaps, Isomap)



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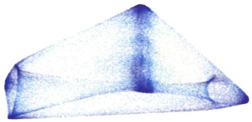

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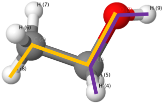
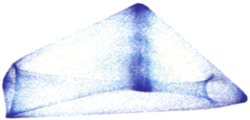
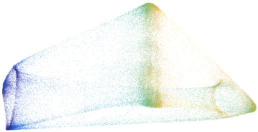
Idea Replace data driven coordinates with selected torsions

- Scientist: proposes a dictionary $\mathcal{G}$ with all variables of interest
- ML algorithm: outputs embedding ϕ,
- ManifoldLasso: finds new coordinates in $\mathcal{G}$ "equivalent" with ϕ $\leftarrow$ our algorithm

▶ Explanation
  ▶ $=$ find manifold coordinates from among scientific variables of interest
  ▶ in the language of the domain

scientific language (torsions)		data driven coordinates (from DiffMaps, Isomap)		coordinates with scientific interpretation (selected torsions)
	$+$		$=$	

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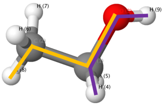

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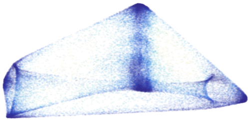

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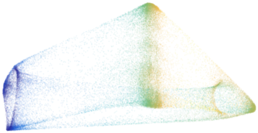

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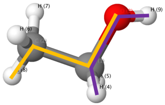
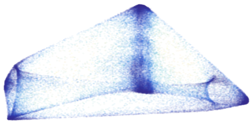


$\mathcal{G} = \{\text{functions } g\}$

$+$

data driven coordinates (from DiffMaps, Isomap)



ϕ

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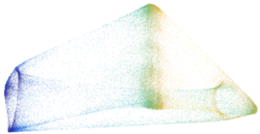
coordinates with scientific interpretation (selected torsions)



$\{g_{j_1}, \ldots g_{j_d}\} \equiv g_S \subset \mathcal{G}$

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Idea: Sparse regression in function space

$$\underset{\text{manifold coordinates}}{\phi} = \overset{\text{homeomorphism}}{h} \circ \underset{\substack{\text{functions from } \mathcal{G} \\ \text{(new coordinates)}}}{g_S}$$

$$D\phi = DhDg_S$$

Leibnitz Rule

Challenges

- sparse, non-linear regression problem
- ML coordinates ϕ defined up to diffeomorphism
- hence, h cannot take parametric form
- we cannot choose a basis for h
- will not ϕ_k depends on single g_j
- will not assume ϕ isometric

- sparse linear regression problem
- For every data i
  - $Y_i = \operatorname{grad} \phi(\xi_i)$,
  - $\mathbf{X}_i = \operatorname{grad} g_{1:p}(\xi)$
  - $\beta_{ij} = \frac{\partial h}{\partial g_j}(\xi_i)$
  - Sparse linear system $Y_i = \mathbf{X}_i\beta_i$
- Constraint: subset S is same for all i

Functional (Group) Lasso

- optimize

$$\min_{\beta} J_\lambda(\beta) = \frac{1}{2}\sum_{i=1}^{n} ||Y_i - \mathbf{X}_i\beta_i||_2^2 + \lambda \sum_j ||\beta_j||, \quad (\textsc{ManifoldLasso})$$

- support S of β selects $g_{j_1,\ldots j_s}$ from $\mathcal{G}$

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manifold coordinates — functions from $\mathcal{G}$ (new coordinates)

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ManifoldLasso Algorithm

Given Data $\xi_{1:n}$, $\dim \mathcal{M} = d$, embedding $\phi(\xi_{1:n})$, dictionary $\mathcal{G} = \{g_{1:p}\}$

1. Estimate tangent subspace at ξ_i by (weighted) PCA
2. Project dictionary functions gradients ∇g_j on tangent subspace, obtain $\mathbf{X}_{1:n} \in \mathbb{R}^{d \times p}$
3. Estimate gradients of $\phi_{1:k}$, obtain $Y_{1:n} \in \mathbb{R}^{d \times m}$

   By pull-back from embedding space ϕ
4. Solve GroupLasso($Y_{1:n}$, $\mathbf{X}_{1:n}$, d), obtain support S

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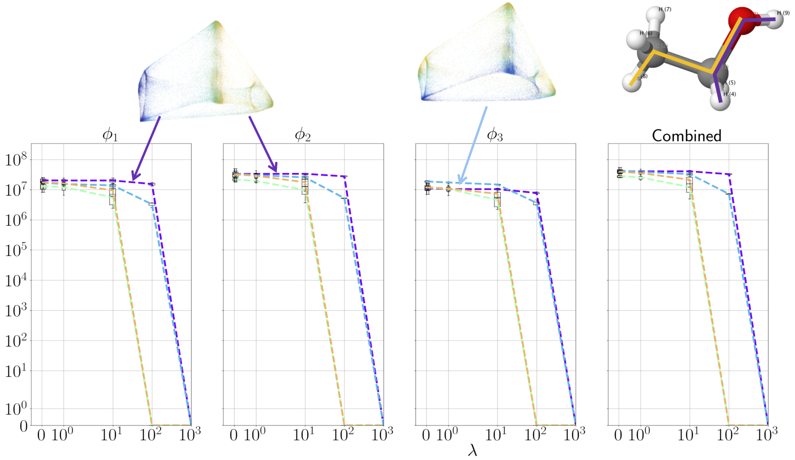
Ethanol MD simulation



regularization paths $\beta_{1:p}$ vs λ

Theory

- When is S unique? / When can $\mathcal{M}$ be uniquely parametrized by $\mathcal{G}$?
  Functional independence conditions on dictionary $\mathcal{G}$ and subset $g_{j_1,\ldots j_s}$
- Basic result

  $f_S = h \circ f_{S'}$ on U iff

$$\operatorname{rank}\begin{pmatrix} Df_S \\ Df_{S'} \end{pmatrix} = \operatorname{rank} Df_{S'} \quad \text{on } U$$

- When can GLasso recover S ?
  (Simple) Incoherence Conditions

$$\mu = \max_{i=1:n, j\in S, j'\notin S} \frac{|\mathbf{X}_{ji}^T \mathbf{X}_{j'i}|}{||\mathbf{X}_{ji}||\,||\mathbf{X}_{j'i}||} \quad \nu = \frac{1}{\min_{i=1:n} ||\mathbf{X}_{iS}^T \mathbf{X}_{iS}||_2} \quad nd\sigma^2 = \sum_{i,k} \epsilon_{ik}^2$$

Theorem If, $||\mathbf{X}_{1:p}|| = 1$, $\mu\nu\sqrt{d} + \frac{\sigma\sqrt{nd}}{\lambda} < 1$ then $\beta_j = 0$ for $j \notin S$.

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- When can GLasso recover S ?
  (Simple) Incoherence Conditions

$$\mu = \max_{i=1:n, j \in S, j' \notin S} \frac{|\mathbf{X}_{ji}^T \mathbf{X}_{j'i}|}{\|\mathbf{X}_{ji}\| \|\mathbf{X}_{j'i}\|} \quad \nu = \frac{1}{\min_{i=1:n} ||\mathbf{X}_{iS}^T \mathbf{X}_{iS}||_2} \quad nd\sigma^2 = \sum_{i,k} \epsilon_{ik}^2$$

<u>Theorem</u> If, $\|\mathbf{X}_{1:p}\| = 1$, $\mu\nu\sqrt{d} + \frac{\sigma\sqrt{nd}}{\lambda} < 1$ then $\beta_j = 0$ for $j \notin S$.

Recovery for ManifoldLasso

Theorem 7 (Support recovery) *Assume that equation (30) holds, and that* $\sum_{i=1}^{n} ||x_{ij}||^2 = \gamma_j^2$ *for all* $j = 1 : p$. *Let* $\gamma_{\max} = \max_{j \notin S} \gamma_j$, $\kappa_S = \max_{i=1:n} \frac{\max_{j \in S} \|x_{ij}\|}{\min_{j \in S} \|x_{ij}\|}$. *Denote by* $\bar{\beta}$ *the solution of (31) for some* $\lambda > 0$. *If* $1 - (s-1)\mu > 0$ *and*

$$\gamma_{\max} \left(\frac{\mu}{1-(s-1)\mu} \frac{\kappa_S}{\min_{i=1}^{n} \min_{j' \in S} \|x_{ij'}\|} + \frac{\sigma\sqrt{d}}{\lambda\sqrt{n}} \right) \leq 1 \tag{37}$$

then $\bar{\beta}_{ij} = 0$ *for* $j \notin S$ *and all* $i = 1, \ldots n$.

Corollary 8 *Assume that equation* (31) *and condition (37) hold. Let* $\kappa = \frac{\mu}{1-(s-1)\mu} \frac{\kappa_S}{\min_{i=1}^{n} \min_{j' \in S} \|x_{ij'}\|}$ *and* $\gamma_S = \|\bar{\bar{X}}_S\|$. *Denote by* $\hat{\beta}$ *the solution to problem* (31) *for some* $\lambda > 0$. *If (1)* $\lambda = c\frac{\gamma_{\max}\sigma\sqrt{d}}{1-\kappa\gamma \max}$, $c > 1$, *and (2)* $||\beta_j^*|| > \sigma\sqrt{d}(\gamma_{\max} + \gamma_S) + \lambda(1+\sqrt{s})$ *for all* $j \in S$, *then the support* S *is recovered exactly and*

$$||\hat{\beta}_j - \beta_j^*|| < \sigma\sqrt{d}(\gamma_{\max} + \gamma_S) + \lambda(1+\sqrt{s}) = \sigma\sqrt{d}\gamma_{\max}\left[1 + \gamma_S/\gamma_{\max} + c\frac{1+\sqrt{s}}{1-\kappa\gamma_{\max}}\right] \quad \text{for all } j \in S.$$

TangentSpaceLasso: ManifoldLasso without embedding

Simplification regress basis of $\mathcal{T}_\xi\mathcal{M}$ on gradients of g_j

Proposition 2 (after (**?**)). *Let $\mathcal{F}, f_j$ be dictionary and dictionary functions on the d–dimensional smooth manifold $\mathcal{M}$. Assume $f_j \in C^\ell$ with $\ell \geq d+1$. Suppose $S \subset [p]$, and denote by* $\operatorname{grad} f_S$ *the $\mathbb{R}^{d\times s}$ matrix of concatenated* $\operatorname{grad} f_j : f \in S$*. Then, if there is a subset $S' \subsetneq S$ such that the following rank condition holds globally:*

$$\operatorname{rank}\begin{pmatrix}\operatorname{grad} f_S \\ \operatorname{grad} f_{S'}\end{pmatrix} = \operatorname{rank}\operatorname{grad} f_{S'}\ . \quad (4)$$

Then there exists a function h which is C^ℓ almost everywhere in the image of $f_{S'}(\mathcal{M})$ such that $f_S = h \circ f_{S'}$

$$\mu_S = \sup_{\xi\in\mathcal{M}^\circ, j\in S, j'\notin S} |\mathbf{X}^T_{\{j\},\xi}\mathbf{X}_{\{j'\},\xi}| \quad (5)$$

$$\nu_S = \sup_{\xi\in\mathcal{M}^\circ \alpha\in\mathbb{R}^d:||\alpha||_2=1} \alpha^T(\mathbf{X}^T_{S,\xi}\mathbf{X}_{S,\xi})^{-1}\alpha. \quad (6)$$

Proposition 3. *Assume that*

1. *$\mathcal{M}$ is d–dimensional C^k compact manifold with strictly positive reach.*
2. *Data ξ are sampled from some density p on $\mathcal{M}$ with $p > 0$ all over $\mathcal{M}$.*
3. *$\xi \in \mathcal{M}^\circ$ with probability 1 under p.*

Let S be the 'true' support, $S(\widehat{\mathbf{B}})$ be the support selected by TSLasso*, μ_S and ν_S be defined by (5) and (6), and further assume*

4. *$|S| = d$.*
5. *Df_S has rank d on $\mathcal{M}^\circ$,*
6. *$\mu_S\nu_S d < 1$.*

Then if we adapt the tangent space estimation algorithm in (**?**) *with bandwidth choice $h = O(\log n/(n-1))^d$, with $n \geq ((1-\mu_S\nu_S d)/2\nu_S d)^{d/(k-1)}$ we have*

$$Pr(S(\widehat{\mathbf{B}}) \subset S) \geq 1 - O\left((\frac{1}{n})^{\frac{k}{d}}\right)\ .$$

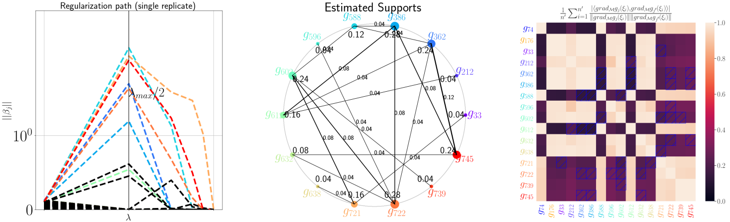
Experiments

Dataset	n	N_a	D	d	ϵ_N	m	n'	p	
SwissRoll	10000	NA	51	2	.18	2	100	51	synthetic
RigidEthanol	10000	9	50	2	3.5	3	100	12	
Ethanol	50000	9	50	2	3.5	3	100	12	skeleton $\mathcal{G}$
Malonaldehyde	50000	9	50	2	3.5	3	100	12	
Toluene	50000	16	50	1	1.9	2	100	30	
Ethanol	50000	9	50	2	3.5	3	100	756	exhaustive $\mathcal{G}$
Malonaldehyde	50000	9	50	2	3.5	3	100	756	
	ϕ						LASSO	$\lvert\mathcal{G}\rvert$	

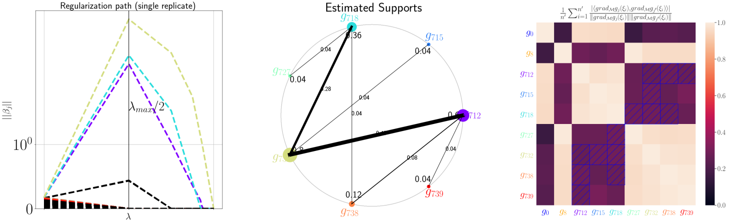
p = dictionary size, m = embedding dimension, n = sample size for manifold estimation, n' = sample size for MANIFOLDLASSO

Two-stage sparse recovery for exhaustive $\mathcal{G}$, $p = 756$

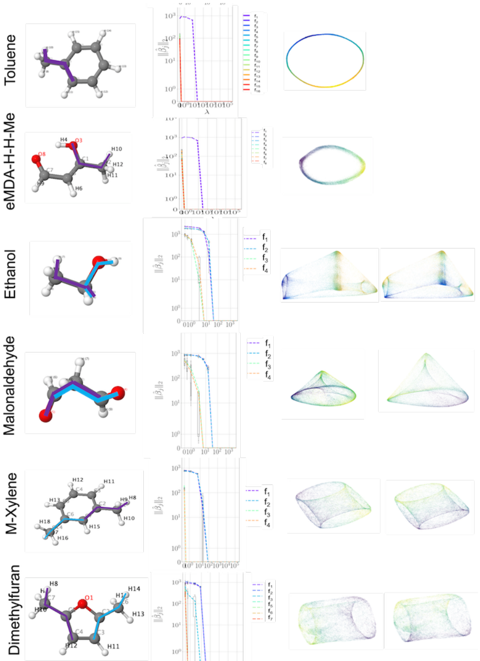
Ethanol



Malonaldehyde



Tangent Space Lasso experiments

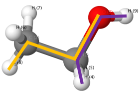


Summary of ManifoldLasso/FunctionalLasso

Technical contribution

- non-linear sparse regression in function spaces
- Method to push/pull vectors through mappings ϕ
- ManifoldLasso: regression of data driven coordinates $\phi_{1:m}$ on domain-specific functions $\mathcal{G} = \{g_{1:p}\}$

scientific language (torsions)



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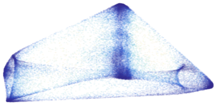
data driven coordinates



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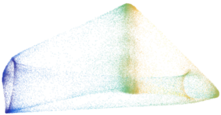
interpretable coordinates



- explains large scale structure with domain-relevant functions
- non-parametric; different from symbolic regression [Brunton et al. 2016, Rudy et al. 2019]
- transmissible knowledge, compare embeddings from different experiments
- extensions: estimated ∇g, simultaneous explanation of multiple manifolds

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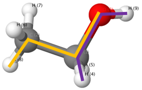

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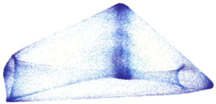

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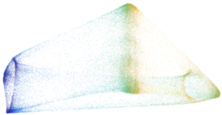

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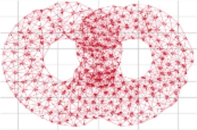
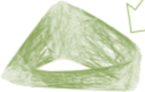
Learning with flows and vector fields [with Yu-chia Chen, Yoannis Kevrekidis]

Directed graph embedding
Manifold + vector field [NIPS 2011]

1-Laplacian estimation
[Arxiv:2103.07626]

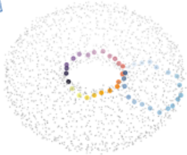


Helmholtz-Hodge
decomposition



Smoothed vector fields

Independent loops
[Arxiv:2107.10970]
[NeurIPS 2021]



Outline

Why Laplacians? Why higher order?

The Laplacian $\mathcal{L}_0 \in \mathbb{R}^{n \times n}$ is central to Manifold Learning

- embedding data by Diffusion Maps [Coifman, Lafon 2006]
- Spectral Clustering

- $\mathcal{L}_0$ related to Riemannian metric – captures geometry of $\mathcal{M}$
- Function approximation
- Smoothing, semi-supervised learning (Laplacian regularization) on manifolds

Higher order Laplacians $\Delta_1, \ldots \Delta_k$ also capture geometry and topology of $\mathcal{M}$

This talk

- estimate first order Laplacian (Helmholtzian) $\mathcal{L}_1(\mathcal{M})$ from data
- calculate Helmholtz-Hodge decomposition of $\mathcal{L}_1(\mathcal{M})$ from data
- Smoothing, function approximation, semi-supervised learning (Laplacian regularization) for vector fields on manifolds
- Manifold prime decomposition ($\approx$ Spectral clustering)
- find short loop bases

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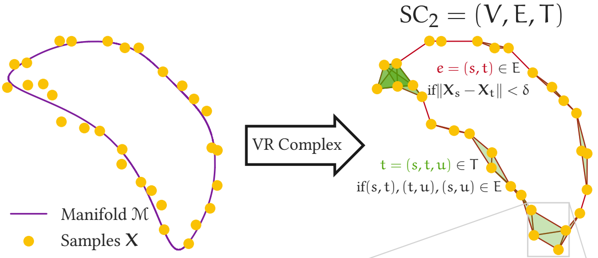
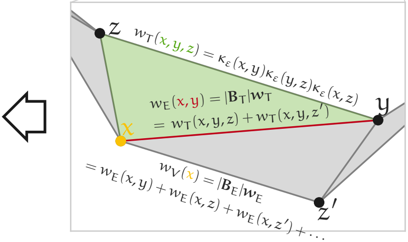
Estimating the 1-Laplacian with samples from $\mathcal{M}$

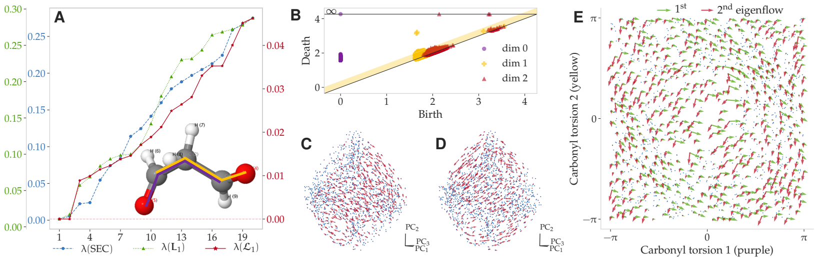


$$\mathcal{L}_1^{\text{down}} = \mathbf{B}_E^\top \boldsymbol{W}_V^{-1} \mathbf{B}_E \boldsymbol{W}_E$$
$$\mathcal{L}_1^{\text{up}} = \boldsymbol{W}_E^{-1} \mathbf{B}_T \boldsymbol{W}_T \mathbf{B}_E^\top$$
$$\Downarrow$$
$$\mathcal{L}_1 = a \cdot \mathcal{L}_1^{\text{down}} + b \cdot \mathcal{L}_1^{\text{up}}$$



$$\boxed{\mathcal{C}_1 \cong \mathbb{R}^{n_E} = \text{gradient} \oplus \text{harmonic} \oplus \text{curl}}$$

$\mathcal{L}_1$ estimation for Molecular Dynamics data (malonaldehyde)



graph Laplacian $w_t = 1$, [Berry, Giannakis 2020], [Chen,M,Kevrekidis 2020]

Outline

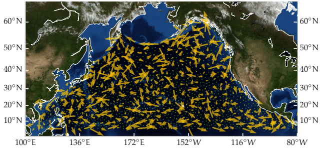
Eigenfunctions of $\mathcal{L}_1$ – what are they useful for?

- Helmholtz-Hodge Decomposition classifies eigenfunctions of $\mathcal{L}_1$

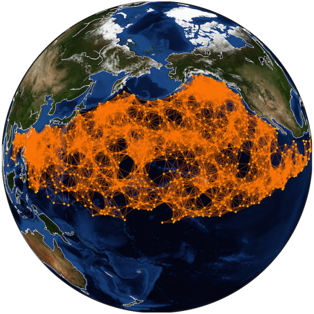
$$\mathcal{C}_1 \cong \mathbb{R}^{n_E} \cong \underbrace{\mathrm{Im}\,\mathcal{L}_1^{\mathrm{down}}}_{\text{gradient}} \oplus \underbrace{\mathrm{Null}\,\mathcal{L}_1}_{\text{harmonic}} \oplus \underbrace{\mathrm{Im}\,\mathcal{L}_1^{\mathrm{up}}}_{\text{curl}}$$

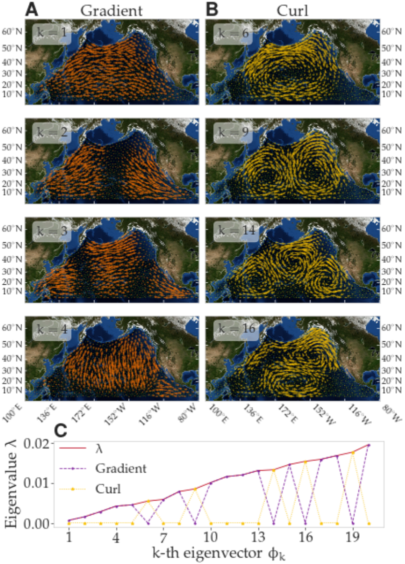
- Analysis of vector fields on $\mathcal{M}$
  - Decompose onto harmonic, gradient, curl
  - Smooth, predict, extend, complete a flow
- Analysis of $\mathcal{M}$
  - $\mathcal{H}_1 = Null\mathcal{L}_1$ Space of loops on $\mathcal{M}$ (1st co-homology space)
  - $\dim \mathcal{H}_1 = \beta_1$ number of (independent loops)
  - Find shortest loop basis

Helmholtz-Hodge decomposition for ocean buoys data

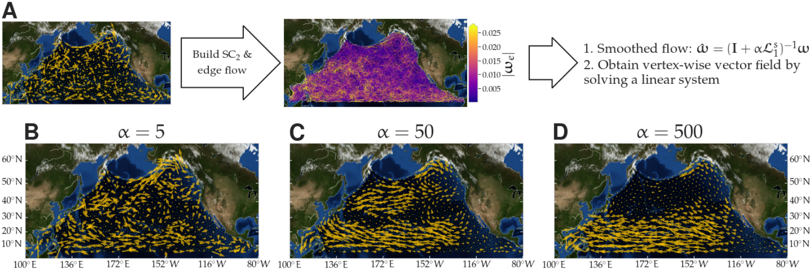


simplicial complex (V, E, T)

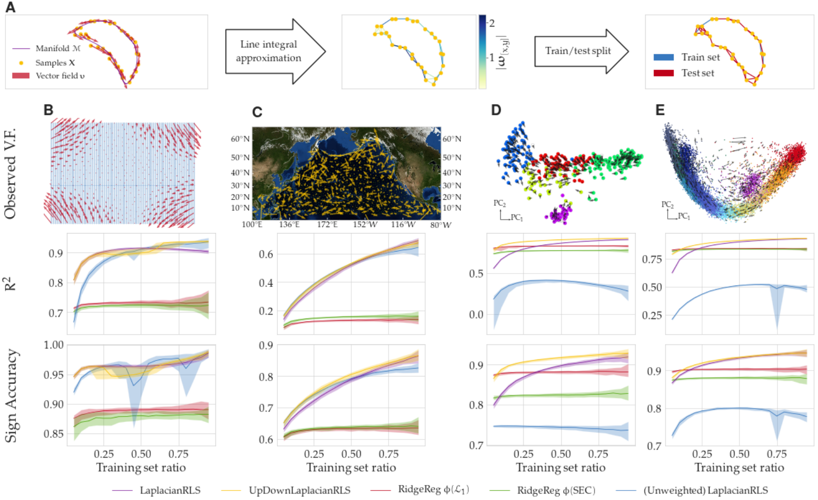




Flow Smoothing



Flow Completion – Semi-Supervised Learning (SSL)



Outline

Manifold coordinates with Scientific meaning

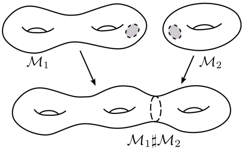
Machine Learning 1-Laplacians, topology, vector fields

- 1-Laplacian $\Delta_1(\mathcal{M})$ estimation from samples
- Analysis of vector fields – Helmholtz-Hodge decomposition
- Harmonic Embedding Spectral Decomposition Algorithm
- Spectral Shortest Homologous Loop Detection

Connected sum and manifold (prime) decomposition

The connected sum **?** $\mathcal{M} = \mathcal{M}_1 \sharp \mathcal{M}_2$:

1. removing two d-dimensional "disks" from $\mathcal{M}_1$ and $\mathcal{M}_2$ (shaded area)
2. gluing together two manifolds at the boundaries



Existence of prime decomposition: factorize a manifold $\mathcal{M} = \mathcal{M}_1 \sharp \cdots \sharp \mathcal{M}_\kappa$ into $\mathcal{M}_i$'s so that $\mathcal{M}_i$ is a prime manifold

- $d = 2$: classification theorem of surfaces **?**
- $d = 3$: the uniqueness of the prime decomposition was shown by Kneser-Milnor theorem **?**
- $d \geq 5$: **?** proved the existence of factorization (but they might not be unique)

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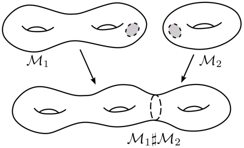

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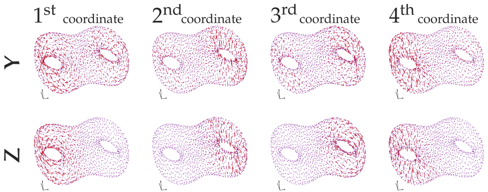
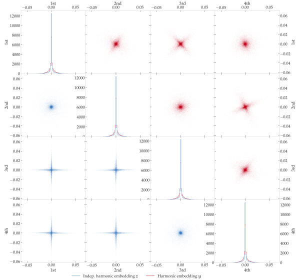
The decomposition of the higher-order homology embedding constructed from the k-Laplacian [Chen,M NeurIPS 2021]

- $\mathcal{L}_1$ is $n_E \times n_E$, operates on edges flows of neighborhood graph
- Null $\mathcal{L}_1 = \mathcal{H}_1$ harmonic space, $\beta_1 = dim\mathcal{H}_1$
- **Y** is basis of $\mathcal{H}_1$ harmonic flows
- **Y** NOT UNIQUE

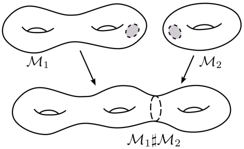
Harmonic Eigenfunctions Y (raw) vs. Z (decoupled)





Connected sum as a matrix perturbation: Assumptions

1. Points are sampled from a decomposable manifold
   - κ-fold connected sum: $\mathcal{M} = \mathcal{M}_1 \sharp \cdots \sharp \mathcal{M}_\kappa$
   - $\mathcal{H}_k(\mathrm{SC})$ (discrete) and $H_k(\mathcal{M}, \mathbb{R})$ (continuous) are isomorphic. Also for every $\mathcal{M}_i$
     - Works for any consistent method to build $\mathcal{L}_k$
     - We use our prior work **?** for $\mathcal{L}_1$



2. No k-homology class is created/destroyed during the connected sum
   - If $\dim(\mathcal{M}) > k$, then $\mathcal{H}_k(\mathcal{M}_1 \sharp \mathcal{M}_2) \cong \mathcal{H}_k(\mathcal{M}_1) \oplus \mathcal{H}_k(\mathcal{M}_2)$ **?**
   - *[Technical] The eigengap of $\mathcal{L}_k$ is the min of each $\hat{\mathcal{L}}_k^{(ii)}$:* $\delta = \min\{\delta_1, \cdots, \delta_\kappa\}$

3. Sparsely connected manifold
   - Not too many triangles are created/destroyed during connected sum (for $k = 1$)
   - Empirically, the perturbation is small even when $\mathcal{M}$ is not sparsely connected
   - *[Technical] Perturbations of ℓ-simplex set Σ_ℓ are small (ϵ_ℓ and ϵ'_ℓ are small) for $\ell = k, k-1$*

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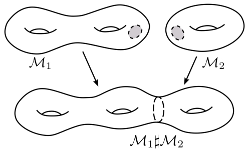

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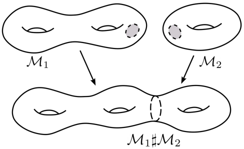
     - We use our prior work **?** for $\mathcal{L}_1$



2. No k-homology class is created/destroyed during the connected sum
   - If $\dim(\mathcal{M}) > k$, then $\mathcal{H}_k(\mathcal{M}_1 \sharp \mathcal{M}_2) \cong \mathcal{H}_k(\mathcal{M}_1) \oplus \mathcal{H}_k(\mathcal{M}_2)$ **?**
   - *[Technical] The eigengap of $\mathcal{L}_k$ is the min of each $\hat{\mathcal{L}}_k^{(ii)}$:* $\delta = \min\{\delta_1, \cdots, \delta_\kappa\}$

3. Sparsely connected manifold
   - Not too many triangles are created/destroyed during connected sum (for $k = 1$)
   - Empirically, the perturbation is small even when $\mathcal{M}$ is not sparsely connected
   - *[Technical] Perturbations of ℓ-simplex set Σ_ℓ are small (ϵ_ℓ and ϵ'_ℓ are small) for $\ell = k, k-1$*

Subspace perturbation

Theorem 1
Under Assumptions 1–3

$$\left\|\mathrm{DiffL}_k^{\mathrm{down}}\right\|^2 \leq \left[2\sqrt{\epsilon_k'} + \epsilon_k' + \left(1+\sqrt{\epsilon_k'}\right)^2 \sqrt{\epsilon_{k-1}'} + 4\sqrt{\epsilon_{k-1}}\right]^2 (k+1)^2; \text{ and}$$

$$\left\|\mathrm{DiffL}_k^{\mathrm{up}}\right\|^2 \leq \left[2\sqrt{\epsilon_k'} + \epsilon_k' + 2\epsilon_k + 4\sqrt{\epsilon_k}\right]^2 (k+2)^2,$$

and there exists a unitary matrix $\mathbf{O} \in \mathbb{R}^{\beta_k \times \beta_k}$ *such that*

$$\left\|\mathbf{Y}_{N_k,:} - \hat{\mathbf{Y}}_{N_k,:}\mathbf{O}\right\|_F^2 \leq \frac{8\beta_k \left[\left\|\mathrm{DiffL}_k^{\mathrm{down}}\right\|^2 + \left\|\mathrm{DiffL}_k^{\mathrm{up}}\right\|^2\right]}{\min\{\delta_1, \cdots, \delta_\kappa\}}. \tag{1}$$

- **Assu. 2:** no topology is destroyed/created
- **Assu. 3:** sparsely connected
- N_k: bound only simplexes that are **not** altered during connected sum

Subspace perturbation

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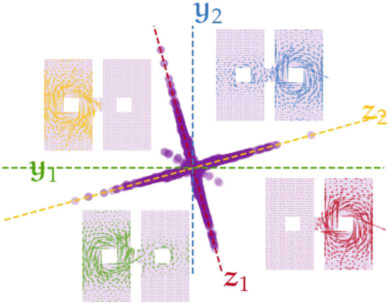
Harmonic Embedding Spectral Decomposition Algorithm

In Simplicial complex (V, E, T), weights $\mathbf{W}_V, \mathbf{W}_E, \mathbf{W}_T$

1. Compute $\mathcal{L}_1$
2. Eigendecomposition
$$\beta_1, \mathbf{Y} \leftarrow Null(\mathcal{L}_1)$$
3. Independent Component Analysis
$$\mathbf{Z} \leftarrow \textsc{ICAnoprewhite}(\mathbf{Y})$$

Out $\mathbf{Z}$



Outline

Manifold coordinates with Scientific meaning

Machine Learning 1-Laplacians, topology, vector fields

- 1-Laplacian $\Delta_1(\mathcal{M})$ estimation from samples
- Analysis of vector fields – Helmholtz-Hodge decomposition
- Harmonic Embedding Spectral Decomposition Algorithm
- Spectral Shortest Homologous Loop Detection

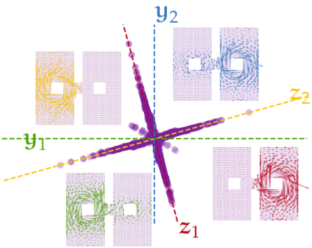
Spectral Shortest Homologous Loop Detection

In $\mathbf{Z} = [\mathbf{z}_1, \ldots \mathbf{z}_{\beta_1}]$, (V, E), edge lengths d_E

for $l = 1 : \beta_1$

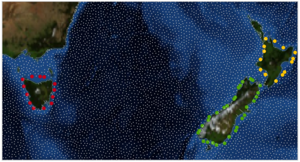
1. Remove edges e with low $|\mathbf{Z}_{le}|$, keep top $1/\beta_1$ fraction E_{keep}
2. Construct $G_l = (V, E_{keep})$, edge weights d_E
3. Repeat for a lot of edges in E_{keep}
   - 3.1 select $e = (t, s_0) \in E_{keep}$
   - 3.2 find shortest path s_0 to t
     $P_e \leftarrow \textsc{Dijkstra}(V, E_{keep} \setminus \{e\}, s_0, t, d_E)$
4. $C_l \leftarrow \text{argmin}_e \, \text{length}(\text{loop}(P_e))$

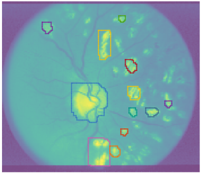
Out loops $C_{1:\beta_1}$

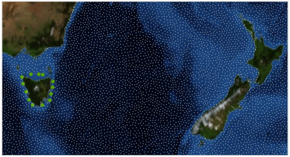


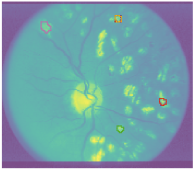
Shortest loop basis on real data

RNA single cell | sculpture | ocean buoys | retina









Summary – Manifold Learning beyond embedding algorithm

- Manifolds, vector fields, ...
  - historically used for modeling scientific data
  - represented analytically

NOW representations learned from data
  - machine learning needs to handle new mathematical concepts
  - need to output results in scientific language

- Generic method for Interpretation in the language of the domain
  - by finding coordinates from among domain-specific functions
  - non-parametric and non-linear
- Extended manifold learning from scalar functions to vector fields
  - first 1-Laplacian estimator
  - continuous limit derived
  - natural extensions of smoothing, semi-supervised learning to vector field data
  - perturbation result for prime manifold decomposition
  - algorithm for shortest loop basis

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Thank you

References I