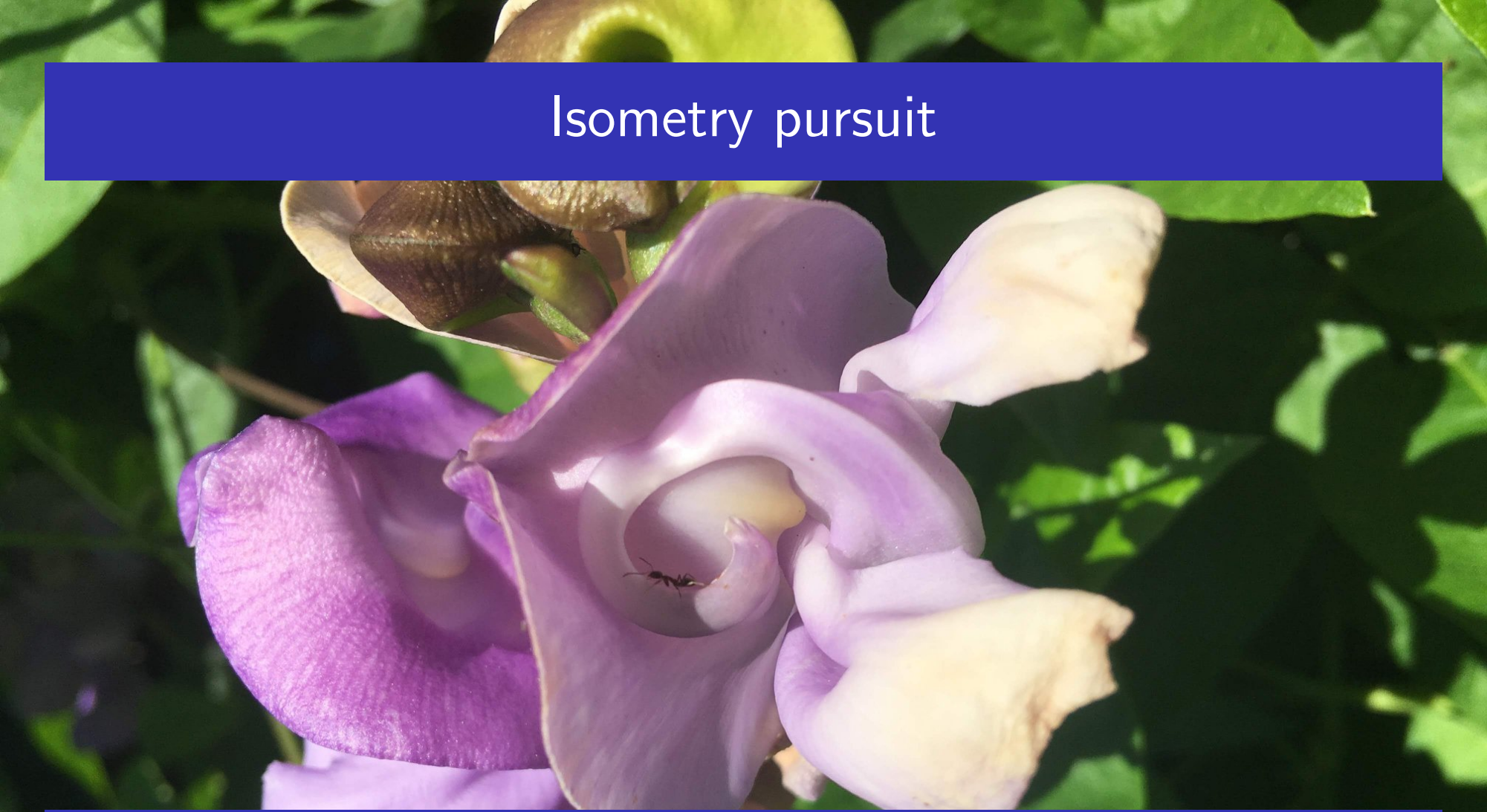
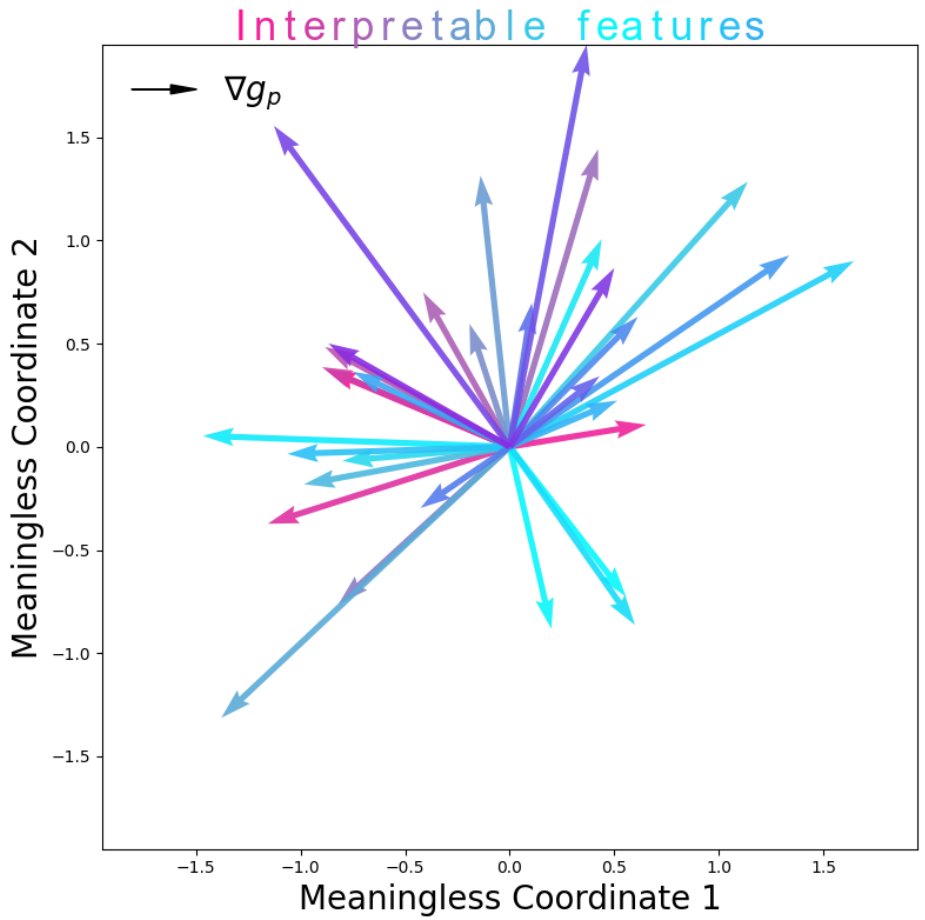
Isometry pursuit



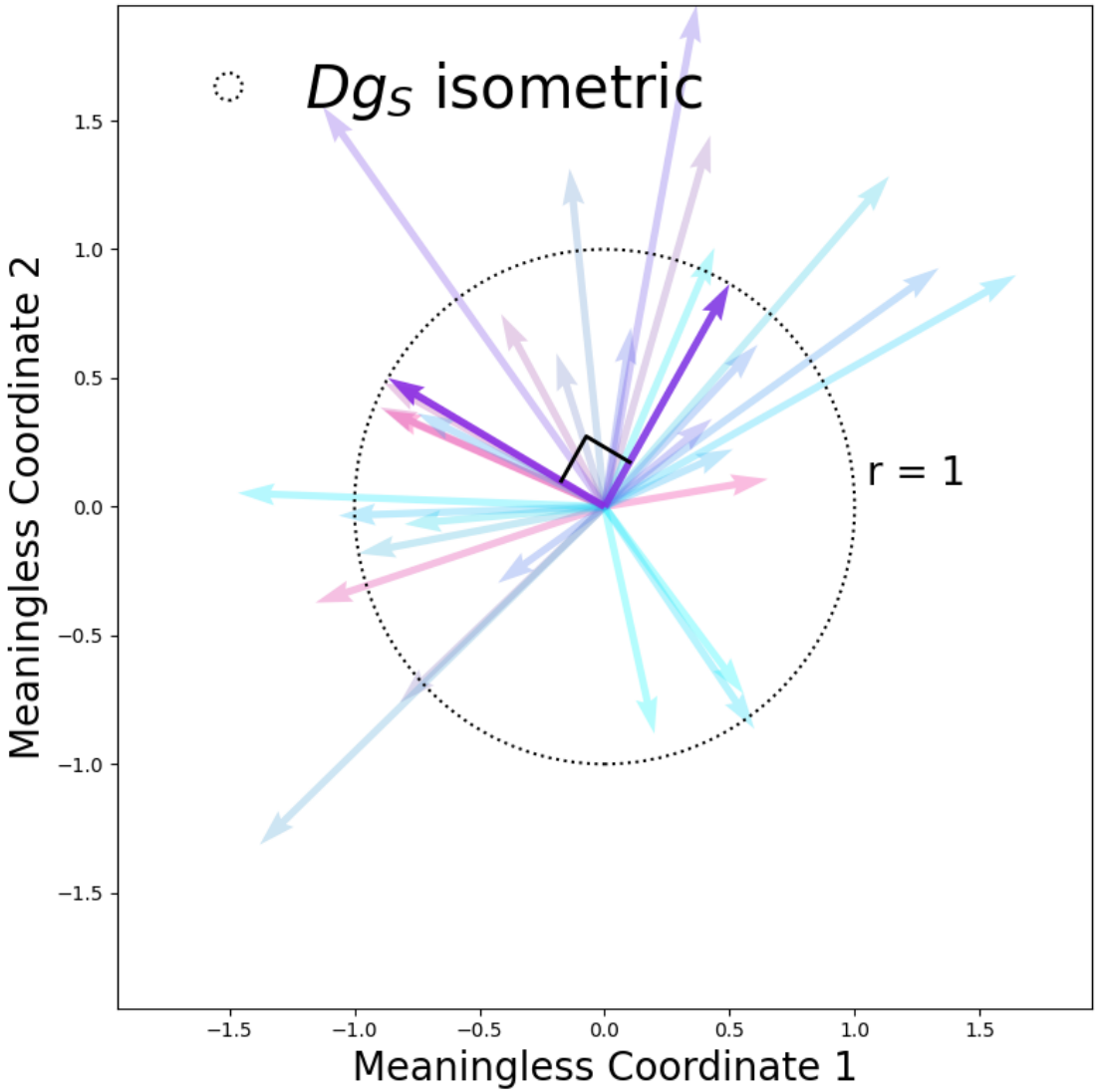
Samson Koelle

December 8, 2024

The problem


Interpretable features
∇g_p
Meaningless Coordinate 2
Meaningless Coordinate 1
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5

Isometry selection



Yet another matrix loss

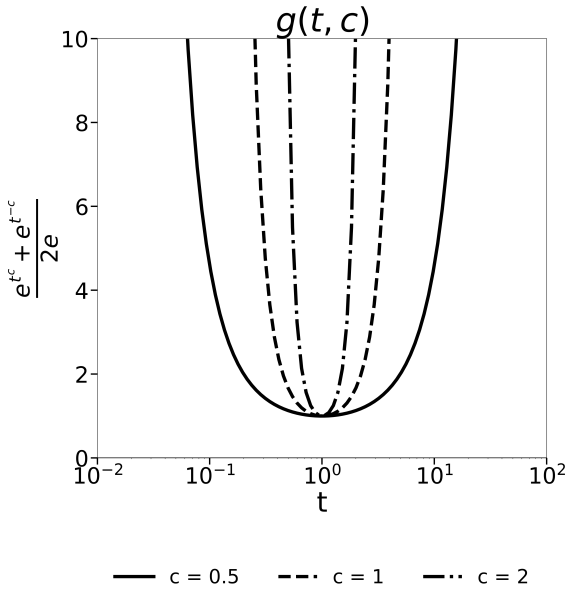
Given a rank D matrix $X \in \mathbb{R}^{D \times P}$ with singular values $\sigma_d \in [D]$, let

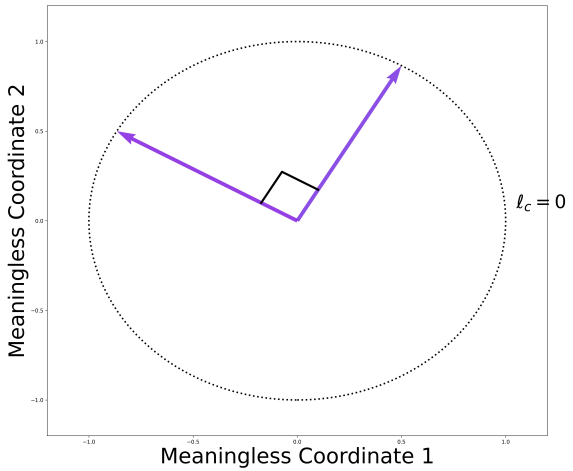
$$\ell_c : \mathbb{R}^{D \times P} \to \mathbb{R}^+$$

$$X \mapsto \sum_{d=1}^{D} g(\sigma_d(X), c) - D$$

$$g : \mathbb{R}^+ \times \mathbb{R}^+ \to \mathbb{R}^+$$

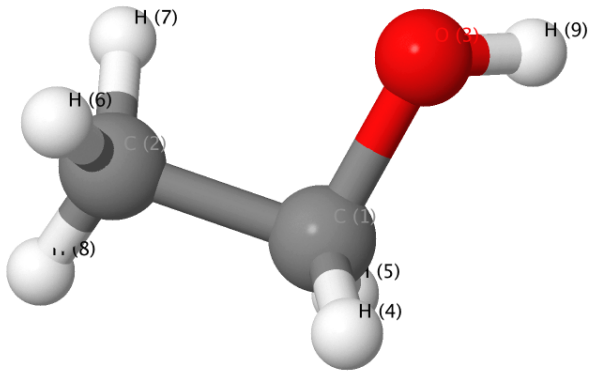
$$(t, c) \mapsto \frac{e^{t^c} + e^{t^{-c}}}{2e}.$$





An application in molecular dynamics simulation (MDS)

- Given a molecule consisting of N_a atoms, simulate T timesteps of molecular motion to generate data $\mathcal{D} \in \mathbb{R}^{T \times 3N_a}$
- These samples concentrate near a low-dimensional manifold which we can estimate using ML



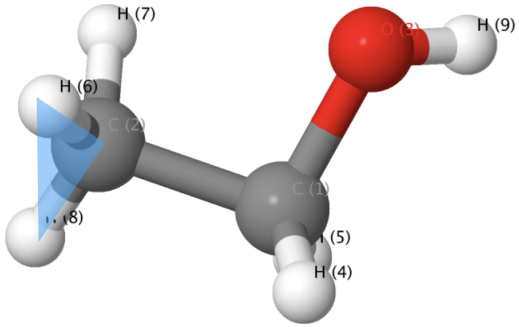
Ethanol ($N_a = 9$) (**Chmiela2018-at**)

Representing invariant geometry

- We featurize each configuration using planar angles prior to ML (**chen2019modern**)

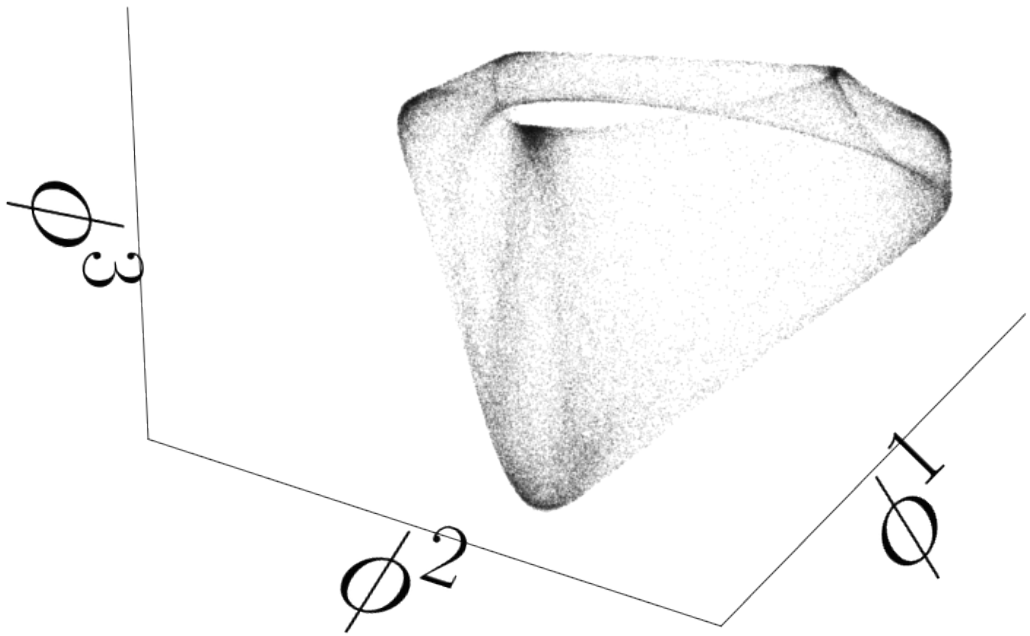
$$\begin{array}{ccccc} \mathbb{R}^{3N_a} & & \mathbb{R}^{3\binom{N_a}{3}} & & \mathbb{R}^{M} \\ \cup & & \cup & & \cup \\ \mathcal{M} & \xrightarrow{\alpha} & \alpha(\mathcal{M}) & \xrightarrow{\phi} & \phi(\alpha(\mathcal{M})) \end{array}$$

α is the planar angle map



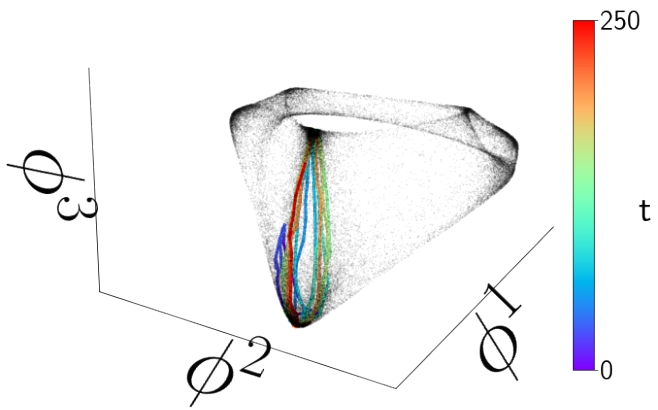
Planar angles are formed by triplets of atoms

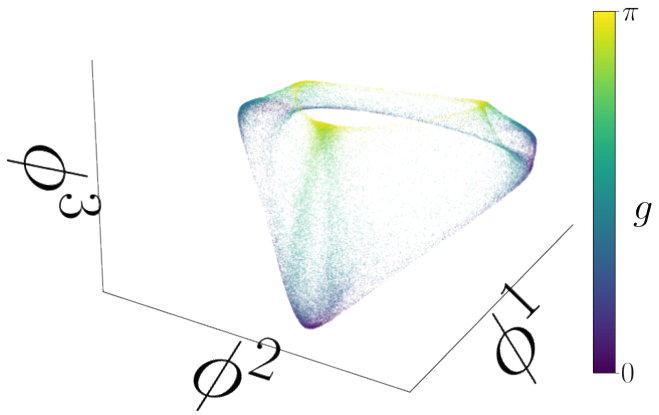
The learned manifold

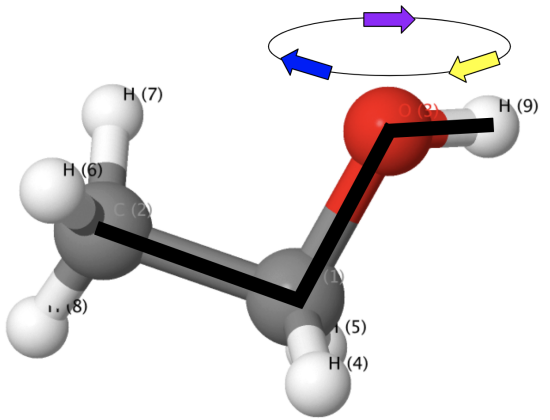


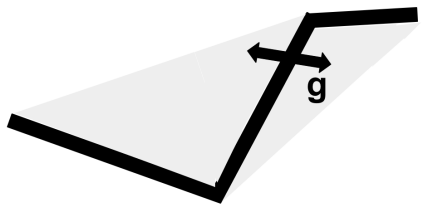
Diffusion Maps embedding of $T = 50000$ ethanol configurations into $M = 3$ dimensions shows a 2 dimensional toroidal molecular manifold

Visually interpreting embeddings







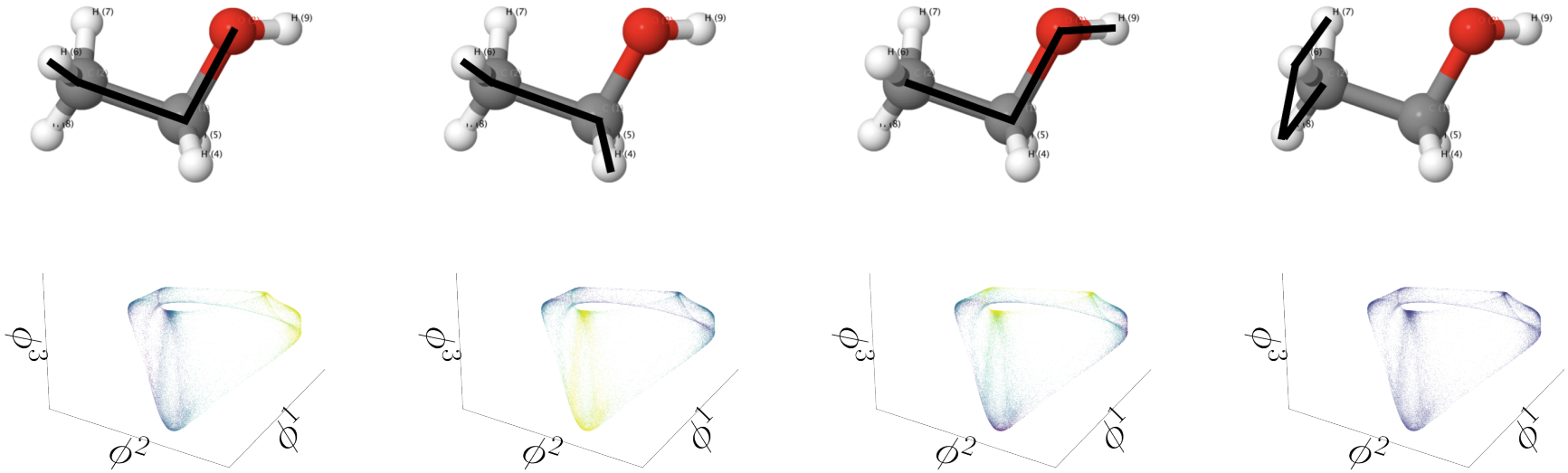


Movement in the ethanol simulation corresponds to hydroxyl rotation

Interpretability is important

- Mechanistic understanding
- Generative control
- Statistical efficiency

Scaling interpretability

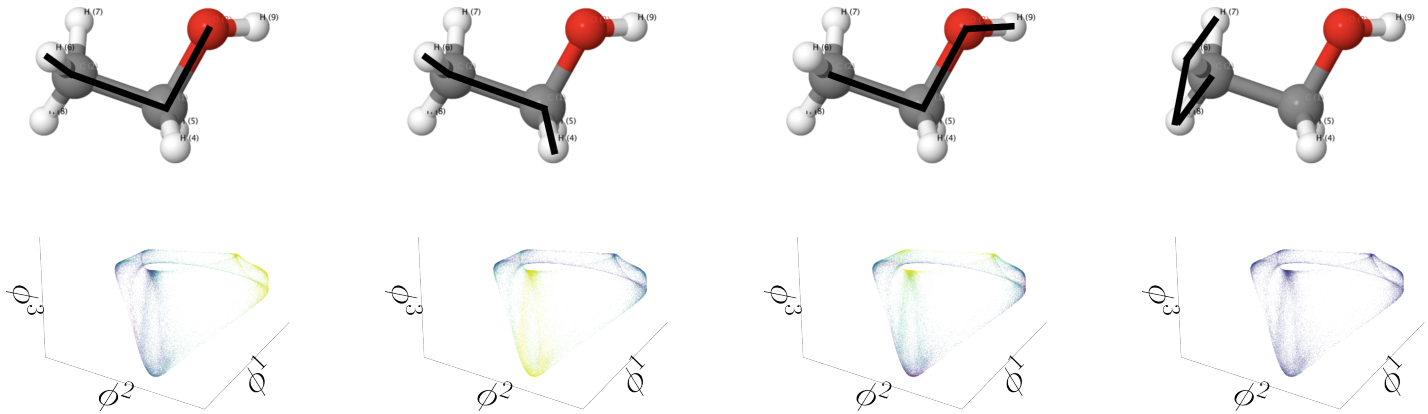


4 of the 756 bond torsions in ethanol

Explanations

Definition (Explanation)

D functions g^p form a *explanation* if their gradients form rank D linear maps from $\mathbb{R}^D \to \mathbb{R}^D$.

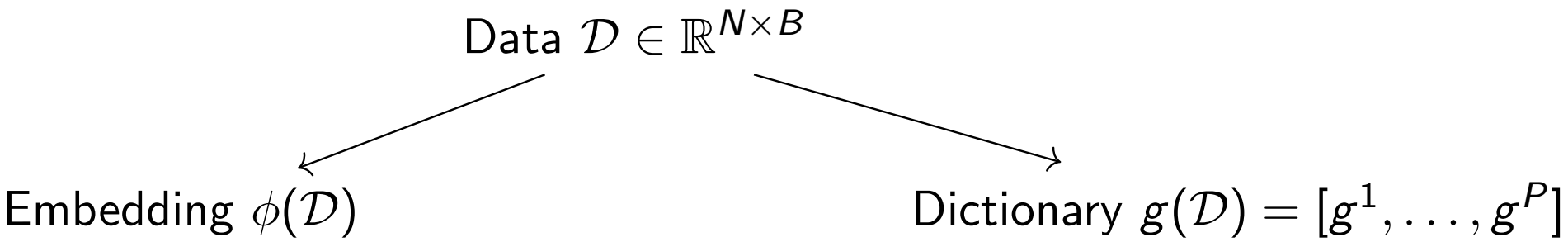


g^1 g^2 g^3 g^4

	g^1	g^2	g^3	g^4
g^1	x	x	✓	x
g^2	x	x	✓	x
g^3	✓	✓	x	x
g^4	x	x	x	x

Are these explanations?

Interpretability examples



Data	**Featurization**	**Embedding**	**Dictionary**	**Explanation**
Configurations	Planar angles	UMAP	Dihedral angles	Methyl rotation
Sentences	Tokens	LLM embeddings	Sparse autoencoder	Time of day
Cells	Gene expression	UMAP	Gene sets	Cell cycle
Galaxies	Spectra	Diffusion maps	Stellar features	Age

Examples of explanations in various scientific domains

Problem statement

- Our goal: find D function subset of g whose gradients w.r.t. $\mathcal{M}$ form a rank D matrix almost everywhere

Proposition (Cut-locus theorem (Sheng2009-ij))

Every manifold $\mathcal{M}$ has an explanation defined everywhere except for a singular set.

- **Koelle2022-oj**: Provide a sparse regression estimator for selecting explanations w.r.t. ϕ
- **Koelle2024-no**: Select explanations without ϕ