On Data Manifolds Entailed by Structural Causal Models

Thomas Melistas

Dominguez-Olmedo, et al. "On Data Manifolds Entailed by Structural Causal Models." ICML, 2023

Overview

- Data Manifolds & Riemannian metric
- A Recap on Structural Causal Models (SCMs)
- Riemannian Manifolds for SCMs
- Application to Counterfactual Explanations

Data Manifolds

- Manifold Hypothesis: *Many high-dimensional real world datasets lie along low-dimensional latent manifolds inside that high-dimensional space*
- The geometric structure of the data manifold is a powerful inductive bias
- Under smoothness conditions, generative models entail data manifolds in which we can use differential geometry & exploit geometric structure for distances, interpolations, etc.

Motivating the use of Riemannian metric (through a VAE case study)

- Points **A** and **B** are in fact closer to each other than **C**, we just measure distance incorrectly!

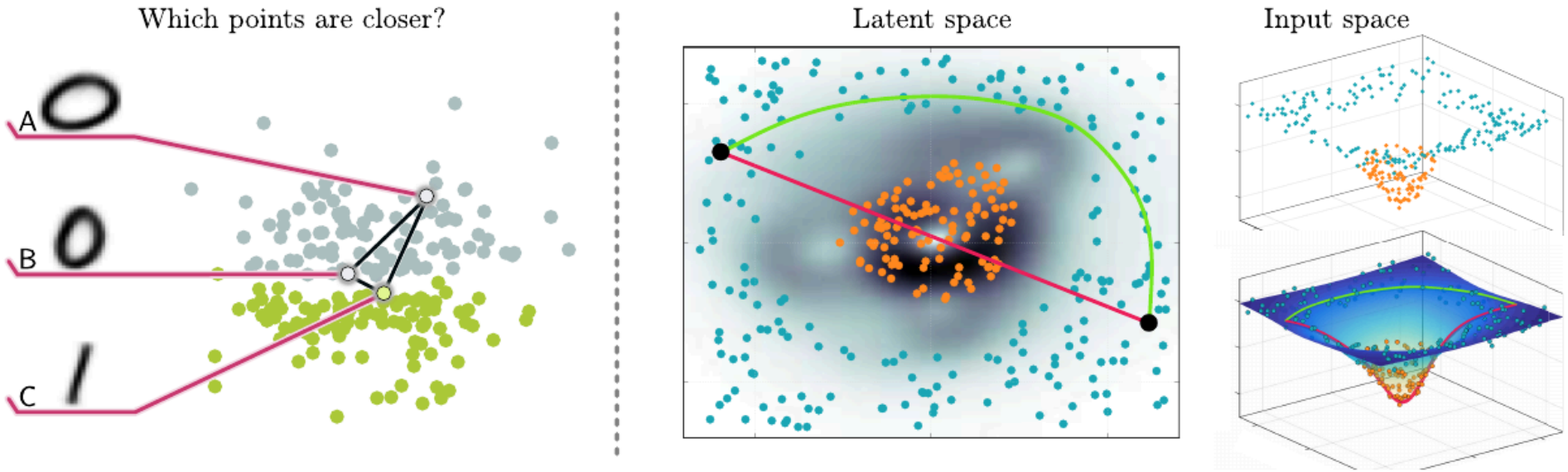
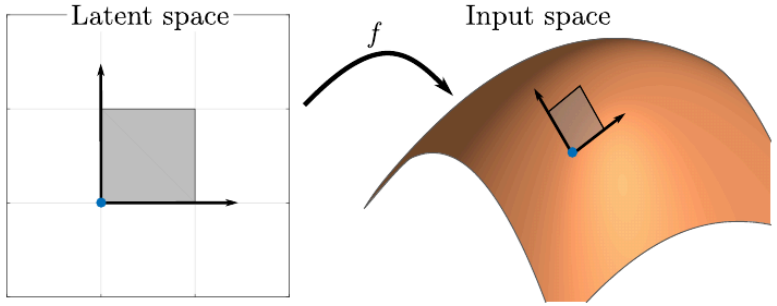


Figure 1: *Left:* An example of how latent space distances do not reflect actual data distances. *Right:* Shortest paths on the surface spanned by the generator do not correspond to straight lines in the latent space, as is assumed by the Euclidean metric.

Arvanitidis, et al. "Latent Space Oddity: On The Curvature Of Deep Generative Models." ICLR, 2018

Motivating the use of Riemannian metric (through a VAE case study)

- $\mathbf{x} \in \mathcal{X}, \mathbf{z} \in \mathcal{Z}$, sufficiently smooth generator $f : \mathcal{Z} \rightarrow \mathcal{X} : \mathbf{x} = f(\mathbf{z})$
- We consider a smooth latent curve: $\gamma_t : [0, 1] \rightarrow \mathcal{Z}$ and we map it to $\mathcal{X}$ through f to measure lengths in input space



- We can find shortest path by solving ODEs that use the Riemannian metric $\mathbf{M}_\gamma = \mathbf{J}_\gamma^{\mathbf{T}} \mathbf{J}_\gamma$, where $\mathbf{J}_\gamma = \left. \frac{\partial f}{\partial \mathbf{z}} \right|_{\mathbf{z}=\gamma}$

Arvanitidis, et al. "Latent Space Oddity: On The Curvature Of Deep Generative Models." ICLR, 2018

Motivating the use of Riemannian metric (through a VAE case study)

- The smoothness assumptions for VAEs involve:
  - twice differentiable activation functions
  - large data dimension (to apply the previous to stochastic generator)
- They use the Riemannian metric for (i) k-means, (ii) interpolations, (iii) different latent probability distribution, (iv) Riemannian random walks

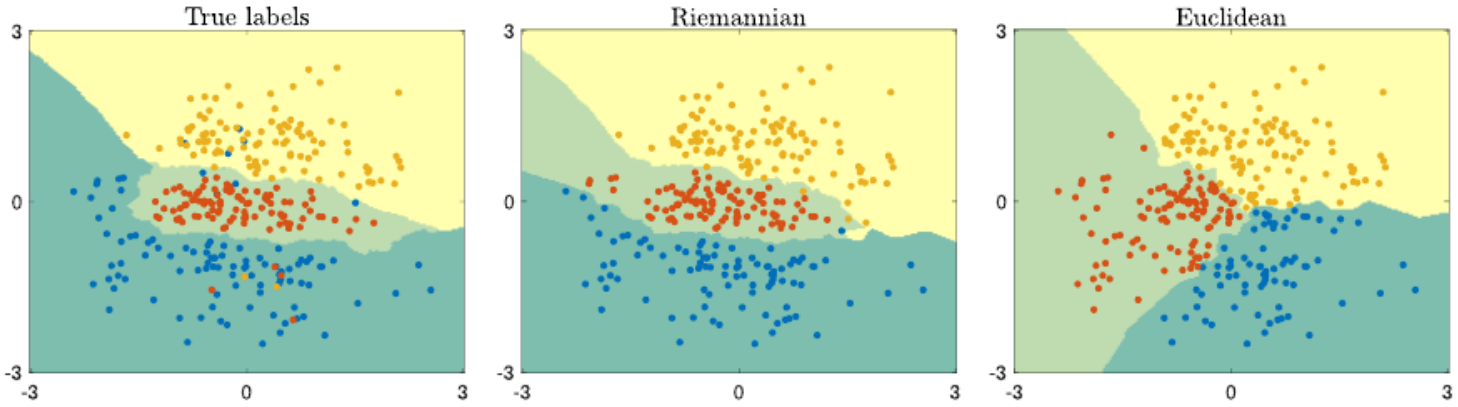


Figure 6: The result of k-means comparing the distance measures. For the decision boundaries we used 7-NN classification.

Arvanitidis, et al. "Latent Space Oddity: On The Curvature Of Deep Generative Models." ICLR, 2018

What is a Riemannian manifold?

- A d-dimensional smooth manifold $\mathcal{M}$ equipped with a Riemannian metric $\mathbf{M} : \mathcal{M} \to \mathcal{S}_{++}^{d},$ with $\mathcal{S}_{++}^{d}$ being a symmetric positive definite matrix
- The length of a smooth curve $\gamma_t : [0,1] \to \mathcal{M}$ is:

$$L(\gamma) = \int_0^1 \sqrt{\dot{\gamma}(t)^T \mathbf{M}(\gamma(t))\dot{\gamma}(t)}dt, \qquad \dot{\gamma}(t) = \frac{d}{dt}\gamma(t)$$

- The Riemannian distance betweeen $p, q \in \mathcal{M}$ is:

$$d_{\mathbf{M}}(p,q) = \inf\{L(\gamma) | \gamma(0) = p, \gamma(1) = q\}$$

- Riemannian volume measure: magnitude of local distortion at $p \in \mathcal{M}$:

$$\mathrm{Vol}_{\mathbf{M}}(p) := \sqrt{\det \mathbf{M}(p)}$$

Pullback metric

- It is used when we do not have a metric for a space
- For a smooth mapping between manifolds $\phi : \mathcal{W} \to \mathcal{M}$, we can define a Riemannian metric for $\mathcal{W}$ as:

$$\mathbf{W}(w) := \mathbf{J}\phi(w)^T \mathbf{M}(\phi(w))\mathbf{J}\phi(w),$$

where $\mathbf{J}\phi(w)$ is the jacobian of ϕ at $w \in \mathcal{W}$

- if ϕ is a diffeomorphism (immersion + injective):

$$d_{\mathbf{W}}(p, q) = d_{\mathbf{M}}(\phi(p), \phi(q))$$

Structural Causal Models

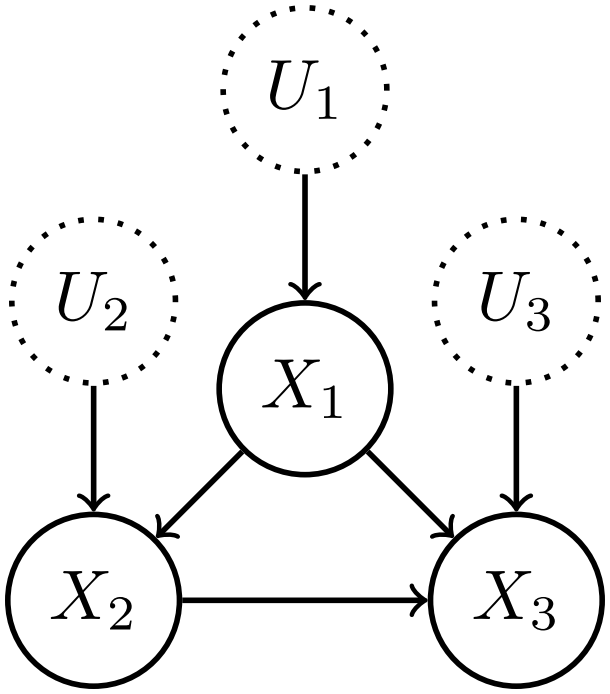
- An SCM $\mathcal{M} := (\mathbf{S}, P_{\mathbf{U}})$ consists of:

(i) structural assignments $\mathbf{S} = \{f_i\}_{i=1}^{d}$, s.t. $X_i := f_i(\mathbf{X}_{pa(i)}, U_i)$,
(ii) a joint distribution $P_{\mathbf{U}}(U_1, \ldots, U_d) = \prod_{i=1}^{d} P(U_i)$ over mutually independent noise variables

X_i: an **endogenous** variable (observed)
$\mathbf{X}_{pa(i)}$: the parents of X_i (its direct *causes*, endogenous)
U_i: an **exogenous** variable (unobserved)

Structural Causal Models

- X_i is caused by parent variables $\mathbf{X}_{pa(i)}$ and exogenous noise variables U_i
- Since the causal graph is acyclic we can substitute parents recursively and obtain $x = f(u)$ (reduced form mapping)
- The entailed observational distribution is $P_{\mathbf{X}}(\mathbf{X} = x) := P_{\mathbf{U}}(\mathbf{U} = f^{-1}(x))$



Interventional distributions

- Hard interventions $\mathcal{J} := do(\mathbf{X}_{\mathcal{I}} = \theta)$ fix a subset of endogenous variables $\mathcal{I}$ to $\theta \in \mathbb{R}^{|\mathcal{I}|}$, s.t. $\mathbf{S}^{\mathcal{J}} = \theta_i$ for intervened variables
- This entails the interventional distribution $P_{\mathbf{X}}^{\mathcal{J}}$

Counterfactual distributions

- Counterfactuals refer to the efect of a hypothetical intervention $\mathcal{J}$ to an observation x
- To compute the counterfactual, we change the structural assignments $\mathbf{S}^{\mathcal{J}}$ as before, but instead of sampling from $P_{\mathbf{U}}$, we compute the posterior $P_{\mathbf{U}|x}$
- this colapses to a single realization $u = f^{-1}(x)$ and counterfactual x^{CF} (f is invertible)
- To define a distribution, we consider a space of interventions $\mathcal{H} := \{do(\mathbf{X}_{\mathcal{I}} = \theta) | \theta \in \Delta\}$, Δ being the possible interventions

SCMs Entail Smooth Manifolds

- Sufficient conditions for the SCMs to induce observational, interventional and counterfactual smooth manifolds
- All are true for three popular classes of SCMs (restrictred functional classes on $\mathbf{S}$):
  - **Additive noise models** (ANMs): $\mathbf{S} := f_i(\mathbf{X}_{pa(i)}) + U_i$
  - **Post-nonlinear models**: $\mathbf{S} := g_i(f_i(\mathbf{X}_{pa(i)}) + U_i), \quad g_i$ invertible
  - **Location-scale noise models**: $\mathbf{S} := f_i(\mathbf{X}_{pa(i)}) + g_i(\mathbf{X}_{pa(i)})U_i,$ g_i strictly positive

Exogenous space smoothness

- The exogenous space $\mathcal{U}$ is a d-dimensional smooth manifold, *if the support of every P_{U_i} is a d_i-dimensional smooth manifold*, where $d = \sum_i d_i$
- Typical choices for P_{U_i} include Gaussian, Gamma distributions, etc. whose support is an open interval of $\mathbb{R}$, a 1-dimensional smooth manifold

Endogenous space smoothness

- As we showed before, for acyclic SCMs: $\mathcal{X} = f(\mathcal{U})$, we further want:
  - f_i differentiable, $\partial_{U_i} f_i(X_{pa_i}, U_i)$ non vanishing (immersion)
  - $f_i(X_{pa_i}, u_i^{(1)}) \neq f_i(X_{pa_i}, u_i^{(2)}) \; \forall u_i^{(1)} \neq u_i^{(2)}$ (injective)
- Interventions entail $(d - m)$-dimensional smooth manifolds ($m = |\mathcal{I}|$), without additional constraints
- The counterfactual space $\mathcal{X}^{\mathcal{H}|x}$ is a m-dimensional smooth manifold, without additional constraints
  - only causal descendants of intervened variables need to have differentiable f_i
  - no constraints on $\mathbf{U}$

SCMs Entail (Riemannian) Data Manifolds

- In previous VAE example, a locally Euclidian metric is regularized to have large volume measure on sparse feature space $\rightarrow$ Curves crossing low data density regions will have large length
- $\mathcal{U}$ isometric to $\mathcal{X}$ if previous constraints exist
- For any Riemannian metric $\mathbf{M}_{\mathcal{U}}$ exists a pullback $\mathbf{M}_{\mathcal{X}}$ and vice-versa for mapping f

Locally Euclidian in $\mathcal{X}$

- Inductive bias: The exogenous noise $\mathbf{U}$ should be similar if it leads to similar observations (in a locally euclidian sense)
- Intuitively, places more weight in differences in outcomes
- Good choice when noise merely represents stochasticity
- The pullback metric $\mathbf{M}_{\mathcal{U}}$ defines a metric in the exogenous space $\mathcal{U}$ grounded on the observed space $\mathcal{X}$

Locally Euclidian in $\mathcal{U}$

- Inductive bias: The observables $\mathbf{X}$ should be similar if they were produced from similar noise (in a locally euclidian sense)
- Intuitively, places more weight in differences in causes
- To be a meaningful metric, noise must be meaningful itself (e.g. deviation from a trend in ANMs)

Regularizing the Riemannian metric

- We want: large volume measure $\mathrm{Vol}_{\mathbf{M}}(p)$ (magnitude of local distortion at p) in regions with low data density
- The Riemannian metric is scaled as:

$$\mathrm{Vol}_{\lambda_{\mathbf{X}}\mathbf{M}}(x) = \frac{\mathrm{Vol}_{\mathbf{M}}(x)}{\alpha \cdot p_{\mathbf{X}}(x) + \beta},$$

where α, β hyperparameters that determine the local curvature as a function of data density $p_{\mathbf{X}}$

- For the interventional manifold we scale by the density of the interventional $P^{\mathcal{J}}_{\mathbf{X}}$
- For the counterfactual we scale by the observational $p_{\mathbf{X}} \rightarrow$ assumes "realistic" counterfactuals

Arvanitidis, et al. "A prior-based approximate latent Riemannian metric." AISTATS, 2022

Counterfactual Explanations

- Not counterfactuals in the causal sense
- Assume a classifier $h : \mathcal{X} \to 0, 1$
- For a x, s.t. $h(x) = 0$, search for the closest positively classified x':

$$\underset{x' \in \mathcal{X}}{\operatorname{argmin}} \quad d(x, x'), \qquad h(x') = 1$$

- The distance function d encodes desired similarity

Desiderata for counterfactual explanations

- Realistic (supported by observed data):
  - Plausible path of change $x \rightarrow x'$ (important for Algorithmic Recourse [1])
  - We use Riemannian distance for $d \rightarrow$ there exists a *shortest curve*
- Causally grounded:
  - Prior works (i) search for interventions [2] or (ii) use backtracking counterfactuals [3]
    but do not consider data manifold

[1] Poyiadzi, et al. "Feasible and actionable counterfactual explanations." AI, Ethics, Society 2020
[2] Karimi et al. "Algorithmic recourse: from counterfactual explanations to interventions" 2021.
[3] von Kügelgen et al. "Backtracking counterfactuals", CLeaR 2023.

Backtracking on the data manifold

- The structural assignments $\mathbf{S}$ do not change (no interventions), but the exogenous noise variables $\mathbf{U}'$ are modified (conditioned to the initial $\mathbf{U}$)

$$\min_{u \in \mathcal{U}} \quad d(f^{-1}(x), u), \quad \text{s.t.} \quad h(f(u)) = 1$$

- We search along the exogenous space $\mathcal{U}$, using the scaled (with $p_{\mathbf{U}}$) Riemannian distance $d_{\lambda_U \mathbf{M}}$ as d to optimize
- Without loss of generality we can use the pullback metric from $\mathcal{X}$

Causal Algorithmic Recourse on the data manifold

- Interventions are recommended, the following must be optimized:

$$\min_{\mathcal{J} \in \mathcal{H}} \quad d(x, \mathbb{CF}(x, \mathcal{J})), \quad \text{s.t.} \quad h(\mathbb{CF}(x, \mathcal{J})) = 1,$$

where $\mathbb{CF}$ maps factuals to counterfactuals under $\mathcal{J}$ interventions on $\mathbf{X}_{\mathcal{I}}$, and $d(x, \mathbb{CF}(x, do(\mathbf{X}_{\mathcal{I}} = \theta))) = \|x_{\mathcal{I}} - \theta\|$

- We search on counterfactual manifold $\mathcal{X}^{\mathcal{H}|x}$, scaling the Riemannian metric $\mathbf{M}$ (with the observational $p_{\mathbf{X}}$) and taking the pullback $\mathbf{M}'$ via the counterfactual mapping $\mathbb{CF}$
- We use $d_{\mathbf{M}'}$ as d and optimize

How to optimize along the manifold

- Compute Riemannian distances by solving for the geodesic γ^*: $\gamma(0) = u_0, \gamma(1) = u_1$, s.t. $d_{\mathbf{M}}(u_0, u_1) := \mathcal{L}(\gamma^*)$
- We can compute γ^* by solving the ODEs (binary value problem)

Experiments

- Datasets (tabular): COMPAS recidivism, Adult demographic
- Models for assignments: Additive Noise Models (using MLPs with 1 hidden layer)
- Modeling probability density of $\mathbf{U}$ with kernel density estimation
- Linear classifiers & NN classifiers (2 hidden layers)

Baselines

- Wachter [1]: objective function $\min_\delta \lambda \|\delta\|_2 + l(h(x+\delta), 1)$
  l cross-entropy loss, gradually anneald λ
- REVISE [2]: above, but optimization in the latent space of a VAE
- FACE [3]: search on a weighted nearest-neighbor graph
- Karimi [4]: (see algorithmic recourse in previous slide)
- Backtracking [5]: (see backtracking counterfactuals in previous slide)
  euclidian distances in $\mathcal{U}$

[1] Wachter, et al. "Counterfactual explanations without opening the black box: Automated decisions and the gdpr." 2017
[2] Joshi, et al. Towards realistic individual recourse and actionable explanations in black-box decision making systems. 2019.
[3] Poyiadzi, et al. "Feasible and actionable counterfactual explanations." AI, Ethics, Society 2020
[4] Karimi et al. "Algorithmic recourse: from counterfactual explanations to interventions" 2021.
[5] von Kügelgen et al. "Backtracking counterfactuals", CLeaR 2023.

Evaluation metrics

- L_2: l_2 distance between factual and counterfactual
- $L_{\mathcal{U}}$, $L_{\mathcal{X}}$: Riemannian distance where metric is locally Euclidian in $\mathcal{U}$ and scaled by $\lambda_{\mathbf{U}}$ (and $\mathcal{X}$ by $\lambda_{\mathbf{X}}$ respectively)
- $L_{\mathcal{M}}$: Riemannian distance induced by a data manifold constructed using kernel density estimation, with a locally Euclidean metric in feature space

Table 1. Experimental results: Counterfactual examples.

	Linear Classifier								NN Classifier							
	Adult				COMPAS				Adult				COMPAS			
Method	$L_{\mathcal{M}}$	L_2	$L_{\mathcal{U}}$	$L_{\mathcal{X}}$	$L_{\mathcal{M}}$	L_2	$L_{\mathcal{U}}$	$L_{\mathcal{X}}$	$L_{\mathcal{M}}$	L_2	$L_{\mathcal{U}}$	$L_{\mathcal{X}}$	$L_{\mathcal{M}}$	L_2	$L_{\mathcal{U}}$	$L_{\mathcal{X}}$
Wachter	7.38	**1.65**	5.76	5.86	2.47	**0.80**	3.00	2.66	3.83	**1.88**	6.59	6.89	2.90	**0.81**	2.75	2.68
Backtr	3.12	1.69	5.47	6.07	4.11	0.83	2.85	2.80	3.51	1.92	6.40	7.00	2.53	0.85	2.83	2.81
FACE	3.29	1.85	5.50	5.69	2.31	0.85	2.88	2.71	5.01	2.10	7.02	6.78	2.25	0.85	3.73	2.54
REVISE	5.64	2.18	9.02	8.71	2.22	0.92	2.57	2.53	3.87	2.21	6.35	6.46	2.55	0.96	2.83	2.90
Ours $L_{\mathcal{U}}$	2.79	1.71	**3.21**	**3.48**	2.77	0.84	**2.33**	2.33	**3.25**	1.95	**4.02**	4.58	2.74	0.86	2.51	2.52
Ours $L_{\mathcal{X}}$	**2.75**	1.70	3.43	**3.48**	**2.18**	0.81	2.35	**2.27**	3.64	1.94	4.29	**4.36**	**2.19**	0.83	**2.41**	**2.51**

Table 2. Experimental results: Algorithmic recourse.

	Linear Classifier								NN Classifier							
	Adult				COMPAS				Adult				COMPAS			
Method	$L_{\mathcal{M}}$	L_2	$L_{\mathcal{U}}$	$L_{\mathcal{X}}$	$L_{\mathcal{M}}$	L_2	$L_{\mathcal{U}}$	$L_{\mathcal{X}}$	$L_{\mathcal{M}}$	L_2	$L_{\mathcal{U}}$	$L_{\mathcal{X}}$	$L_{\mathcal{M}}$	L_2	$L_{\mathcal{U}}$	$L_{\mathcal{X}}$
Karimi et al.	2.68	**1.49**	4.04	4.05	1.33	**0.75**	2.62	2.63	3.47	**1.84**	5.63	5.66	1.37	**0.79**	2.68	2.69
Ours $L_{\mathcal{U}}$	1.29	1.58	1.48	1.48	1.19	0.79	**2.25**	2.29	**0.86**	1.92	**1.15**	**1.15**	**1.20**	0.85	**2.20**	2.23
Ours $L_{\mathcal{X}}$	**1.09**	1.58	**1.31**	**1.32**	**1.17**	0.79	2.27	**2.27**	1.13	1.91	1.52	1.52	1.22	0.85	2.23	**2.19**

Results

- Closer in $L_{\mathcal{U}}$, $L_{\mathcal{X}}$ as expected
- $L_{\mathcal{M}}$ shows that they generalize despite functional assumptions (ANMs)

Thank you for your attention

Questions

- Would this work with deep mechanisms (i.e. VAE, GAN, Diffusion) for high-dimensional variables (i.e. images)?