Diffeomorphic Counterfactuals

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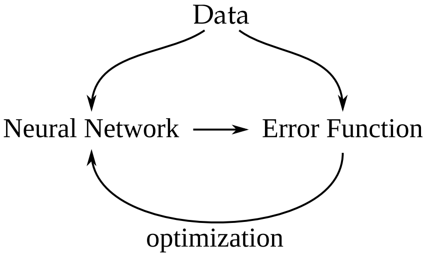
At the interface of physics, mathematics and artificial intelligence

Based on joint work with
Ann-Kathrin Dombrowski, Klaus-Robert Müller and Pan Kessel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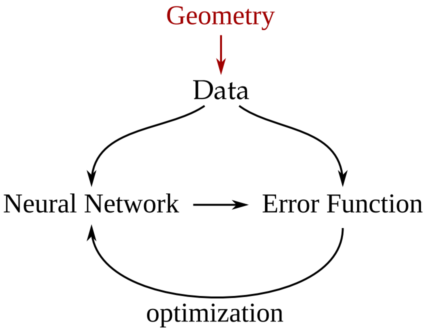
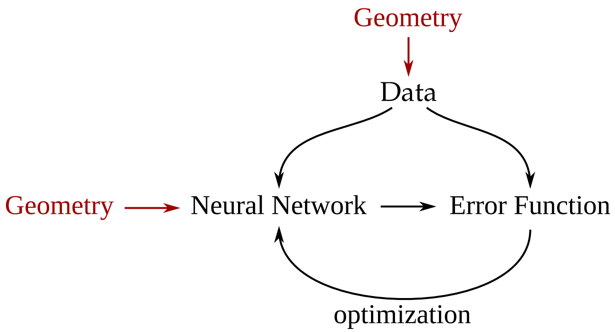
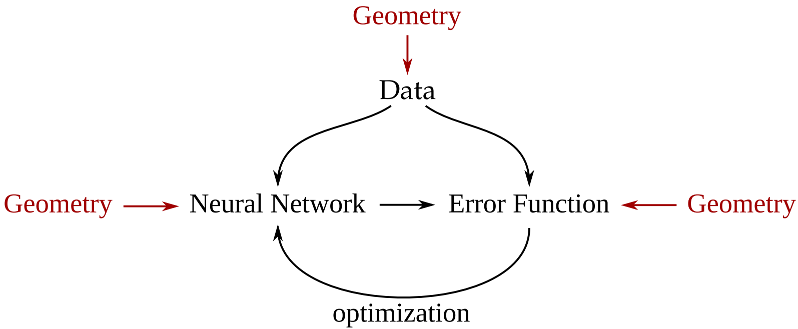
Neural Network
Error Function
optimization

Geometric Deep Learning



Geometric Deep Learning

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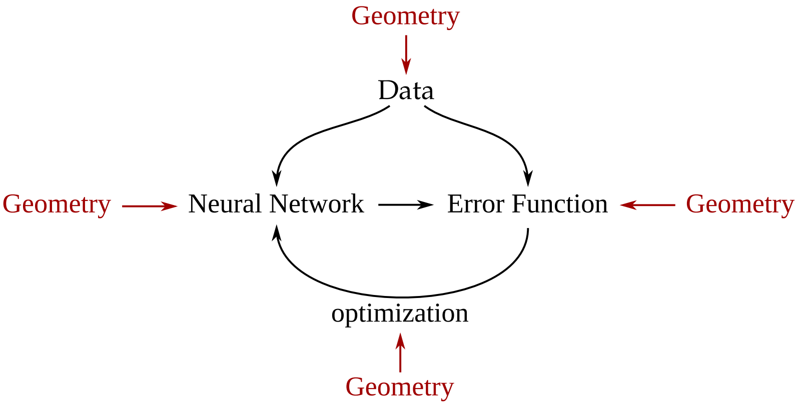
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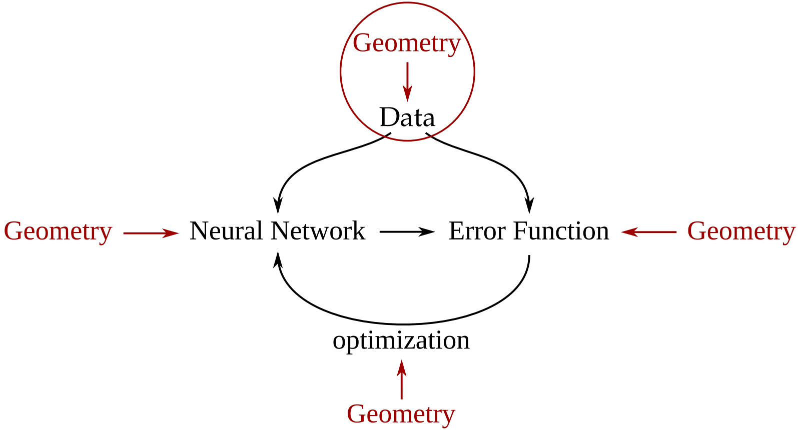
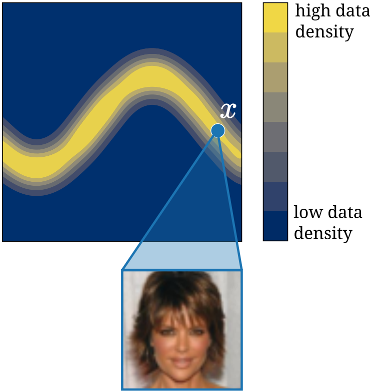
Geometric Deep Learning



Geometry of the training data

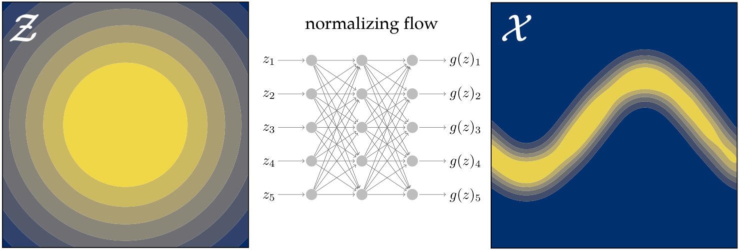


- Manifold Hypothesis: Data lies on low-dim. submanifold of high-dim. input space
- E.g. MNIST pictures lie on ~ 30-dim. submanifold of $28 \times 28 = 784$ dim. input space

Learned diffeomorphisms

[Dinh, Krueger, Bengio, 2014]

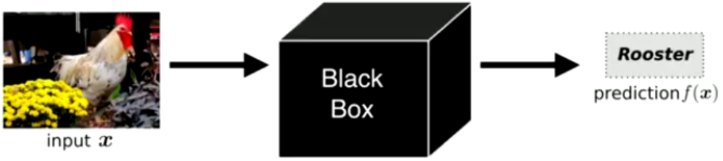
- How to characterize the data manifold?
- Can learn a diffeomorphism between a simple distribution and data distribution



- Diffeomorphism is given by another neural network, a ***normalizing flow***
- Get access to the data manifold in a functional form
- Connections to shape matching [Jansson, Modin, 2022]
- Connections to optimal transport [Chen, Karlsson, Ringh, 2021] [Bauer, Joshi, Modin, 2017] [Onken, Fung, Li, Ruthotto 2020]

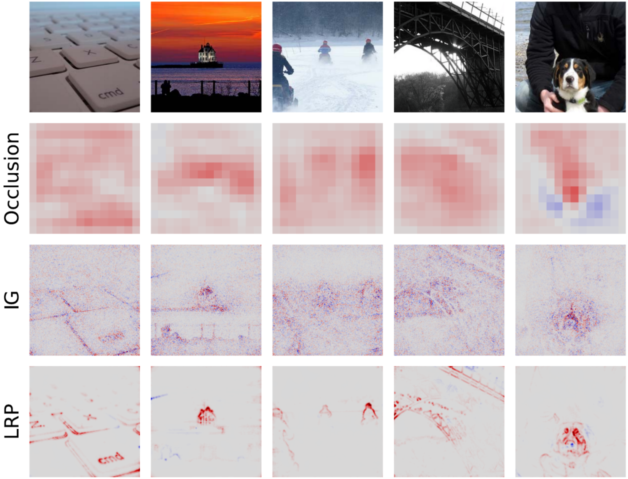
Explainable AI (XAI)

[Review: Samek et al. 2021]



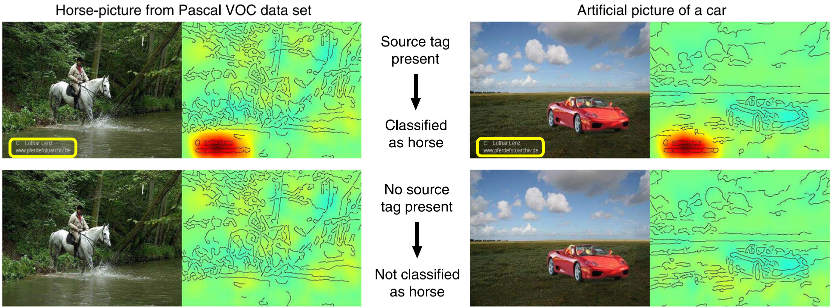
- Neural network classifiers lack inherent interpretability
- This is in contrast to more traditional methods like linear- or physical models
- For safety-critical applications this poses a serious challenge in practice
- Research progress can also be impeded
- Need explanations which provide insight into the neural network decisions

Saliency maps



Clever Hans Effect

[Lapuschkin et al., Nat Commun 2019]

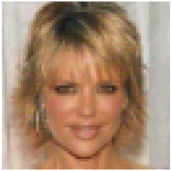


Clever Hans

Counterfactual explanations

- ***Counterfactual of a sample***: Data point close to original but with different classification
- Difference between original and counterfactual reveals features which led to classification
- Example from CelebA dataset, classified as not-blonde:

original x



counterfactual x'

$|x - x'|$

Adversarial Examples

- Small perturbations can lead to misclassifications

$p_{\text{blonde}}\Big($  $\Big) = 0.01$ but $p_{\text{blonde}}\Big($  $\Big) = 0.99$

Adversarial Examples

- Small perturbations can lead to misclassifications

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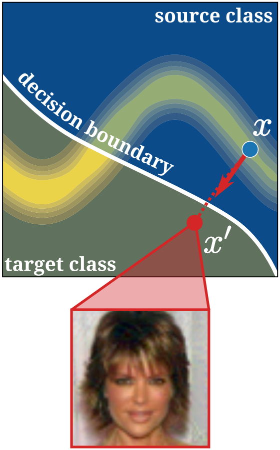
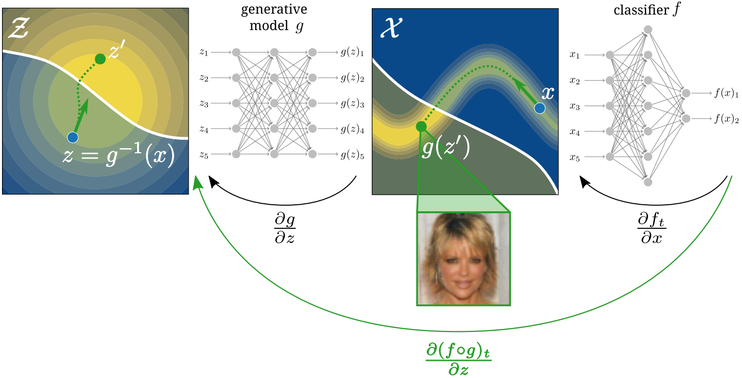
- Reason: Classifier only trained on the data manifold



 [Dombrowski, JG, Müller, Kessel, 2022]

- Can use normalizing flows to optimize along the data manifold ⇒ ***counterfactuals***



$$z^{(i+1)} = z^{(i)} + \lambda \frac{\partial (f \circ g)_t}{\partial z}\left(z^{(i)}\right)$$

Gradient ascent in base space

- Gradient ascent in Z for class k of the classifier f with learning rate λ:

$$z^{(t+1)} = z^{(t)} + \lambda \frac{\partial (f \circ g)_k}{\partial z}(z^{(t)})$$

- Using change-of-variable under the flow:

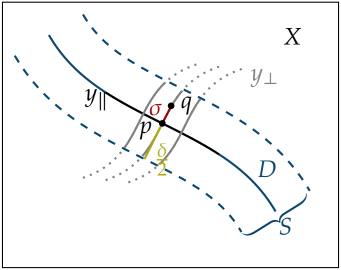
Theorem

Gradient ascent in the base space Z is given by

$$x^{(t+1)} = x^{(t)} + \lambda \, \boldsymbol{\gamma^{-1}(x^{(t)})} \, \frac{\partial f_k}{\partial x}(x^{(t)}) + \mathcal{O}(\lambda^2)$$

where $\gamma^{-1}(x) = \left(\frac{\partial g}{\partial z} \frac{\partial g}{\partial z}^T\right)(g^{-1}(x))$ is the inverse of the induced metric on X from Z under the flow g.

Data coordinates



- Assume that data lies in a region $S = \mathrm{supp}(p)$ around data manifold D, in data coordinates x^α

$$S_x = \left\{ x_D + x_\delta \,\middle|\, x_D \in D_x,\ x_\delta^\alpha \in \left(-\frac{\delta}{2}, \frac{\delta}{2}\right) \right\}$$

with $\delta \ll 1$.

- Define normal coordinates y^μ in a neighborhood of D

Gradient ascent in y-coordinates

- By choosing $\{n_i\}$ orthogonal wrt γ, the inverse induced metric takes the form

$$\gamma^{\mu\nu}(y) = \begin{pmatrix} \gamma_D^{-1}(y) & & & \\ & \gamma_{\perp_1}^{-1} & & \\ & & \ddots & \\ & & & \gamma_{\perp_{N_X - N_D}}^{-1} \end{pmatrix}^{\mu\nu} .$$

- The gradient ascent update $g^\alpha(z^{(i+1)}) = g^\alpha(z^{(i)}) + \lambda\, \gamma^{\alpha\beta} \frac{\partial f_t}{\partial x^\beta} + \mathcal{O}(\lambda^2)$ becomes

$$\gamma^{\alpha\beta} \frac{\partial f_t}{\partial x^\beta} = \frac{\partial x^\alpha}{\partial y_\parallel^\mu} \gamma_D^{\mu\nu} \frac{\partial f_t}{\partial y_\parallel^\nu} + \frac{\partial x^\alpha}{\partial y_\perp^i} \gamma_{\perp_i}^{-1} \frac{\partial f_t}{\partial y_\perp^i}$$

- For $\gamma_{\perp_i}^{-1} \to 0$ and $\frac{\partial x}{\partial y_\perp}$ bounded we have

$$\gamma^{\alpha\beta} \frac{\partial f_t}{\partial x^\beta} \to \frac{\partial x^\alpha}{\partial y_\parallel^\mu} \gamma_D^{\mu\nu} \frac{\partial f_t}{\partial y_\parallel^\nu}$$

and hence the update step points along the data manifold.

$\Rightarrow$ ***In this case, obtain counterfactuals, not adversarial examples!***

The induced metric for well-trained generative models

Theorem (Diffeomorphic Counterfactuals)

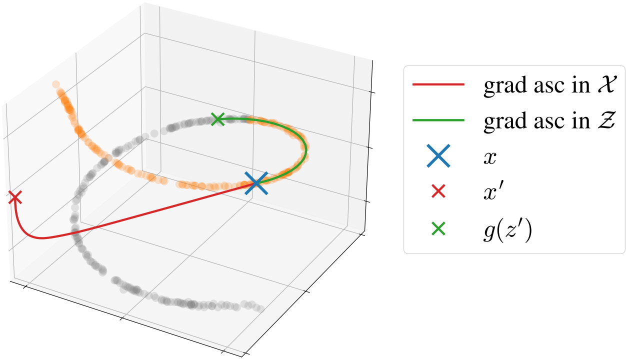
For $\epsilon \in (0, 1)$ and g a normalizing flow with Kullback–Leibler divergence $\mathrm{KL}(p, q) < \epsilon$,

$$\gamma_{\perp_i}^{-1} \longrightarrow 0 \qquad \text{as} \qquad \delta \longrightarrow 0$$

for all $i \in \{1, \ldots, N_X - N_D\}$.

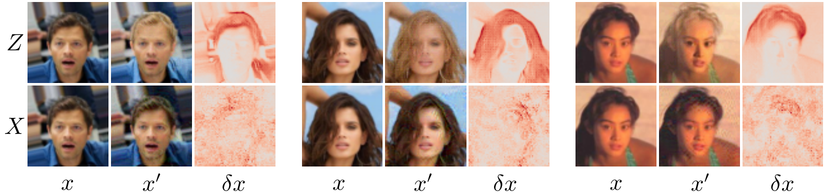
$\Rightarrow$ ***For well-trained generative models, the gradient ascent update in Z stays on the data manifold***

Toy example



Diffeomorphic Counterfactuals with CelebA

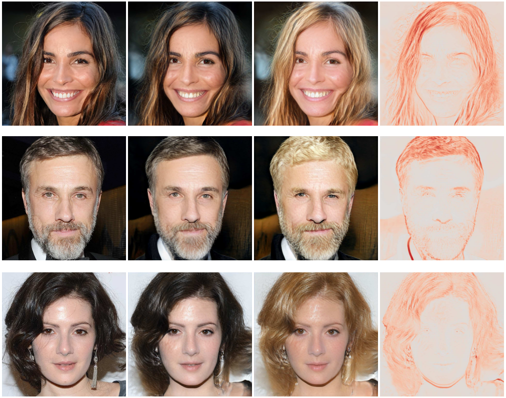
- Classifier: Binary CNN trained on ***blonde/not blonde*** attribute (test accuracy: 94%)
- Flow: Glow [Kingma et al., NeurIPS 2018]
- Task: Change classification from ***not blonde*** to ***blonde***



- Top row: Counterfactual computed in base space
- Bottom row: Adersarial example computed in data space

Approximately Diffeomorphic Counterfactuals with CelebA-HQ

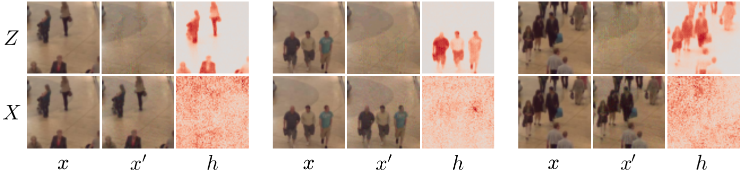
- For general generating models, inversion not exact ($\tilde{x} = g(z_0) \neq x_0$)
- Approximate diffeomorphic counterfactuals can be generated for high-dimensional datasets (1024×1024 pixels for CelebA-HQ)
- Use StyleGAN trained on CelebA-HQ [Karras et al., IEEE/CVF 2019]
- Use HyperStyle inversion of StyleGAN to find initial latent [Alaluf et al., CVPR 2022]



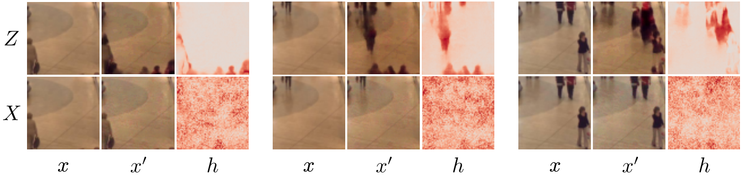
x $\tilde{x}$ $\tilde{x}'$ h

Diffeomorphic Counterfactuals for regression

- Consider crowd-counting dataset of mall images
- Count number of people in the image [Ribera et al., CVPR 2019]
- Flow: Glow [Kingma et al., NeurIPS 2018]
- Optimize for low number of people



- Optimize for high number of people



Diffeomorphic Counterfactuals with Generative Models

arXiv: 2206.05075

Accepted at IEEE PAMI

Thank you!

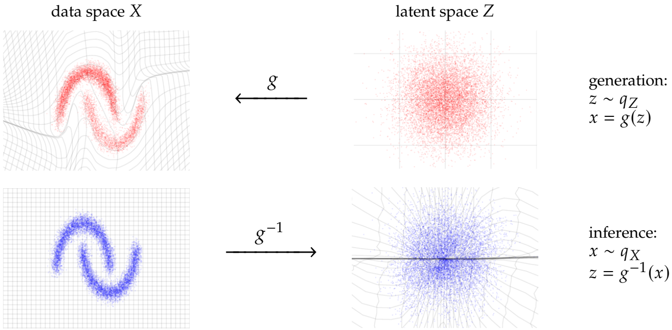
Appendix

Normalizing flows

- Generative model g which maps base space Z to data space X ***bijectively***, i.e. it is a ***diffeomorphism***
- Probability distribution q_Z in Z is simple, e.g. uniform or normal
- Probability distribution q_X in X is given by change of variables

$$q_X(x) = q_Z(g^{-1}(x)) \left| \det \frac{\partial z}{\partial x} \right|$$

- Train by maximizing log-likelihood $\log q_X$ of train data

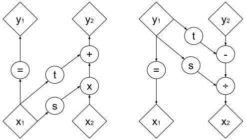


RealNVP

[Dinh et al., ICLR 2017]

- g is realized as a neural network with bijective building blocks
- Network needs to be easily invertible and have a tractable Jacobian determinant
- RealNVP uses ***affine coupling layers***

$$
\begin{aligned}
y_{1:d} &= x_{1:d} \\
y_{d+1:D} &= x_{d+1:D} \odot \exp(s(x_{1:d})) + t(x_{1:d}) \\
s, t &: \mathbb{R}^d \to \mathbb{R}^{D-d} \qquad \text{(deep CNNs)}
\end{aligned}
$$

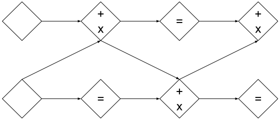


forward backward

- The Jacobian is given by

$$
\frac{\partial y}{\partial x^T} = \begin{bmatrix} \mathbb{1}_d & 0 \\ \frac{\partial y_{d+1:D}}{\partial x_{1:d}^T} & \operatorname{diag}\left(\exp(s(x_{1:d}))\right) \end{bmatrix} \quad \Rightarrow \quad \left|\frac{\partial y}{\partial x^T}\right| = \exp\left(\sum_j s(x_{1:d})_j\right)
$$

- Alternate the parts which are modified from layer to layer



- RealNVP uses multi-scale architecture

The induced metric for well-trained generative models

Theorem (Diffeomorphic Counterfactuals)

For $\epsilon \in (0,1)$ and g a normalizing flow with Kullback–Leibler divergence $\mathrm{KL}(p,q) < \epsilon$,

$$\gamma_{\perp_i}^{-1} \to 0 \qquad \text{as} \qquad \delta \to 0$$

for all $i \in \{1, \ldots, N_X - N_D\}$.

Theorem (Approximately Diffeomorphic Counterfactuals)

If $g : Z \to X$ is a generative model with $D \subset g(Z)$ and image $g(Z)$ which extends in any non-singular orthogonal direction $y_\perp^i$ to regions outside of D of low probability $p(x) \ll 1$,

$$\gamma_{\perp_i}^{-1} \to 0$$

for $\delta \to 0$ for all non-singular orthogonal directions $y_\perp^i$.

$\Rightarrow$ ***For well-trained generative models, the gradient ascent update in Z stays on the data manifold***

Sketch of proof (flow-case)

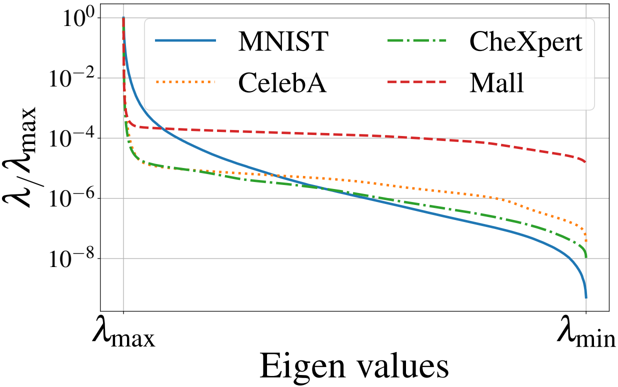
- For flows g with $\mathrm{KL}(p, q) < \epsilon$, almost all probability mass is concentrated in $S = \mathrm{supp}(p)$

$$
\begin{aligned}
0 < 1 - \epsilon < & \int_{S_x} q_X(x)\,\mathrm{d}x \\
= & \int_{S_x} q_Z(g^{-1}(x)) \left| \frac{\partial z^a}{\partial x^\alpha} \right| \mathrm{d}x \\
= & \int_{D_y} \sqrt{|\gamma_D|} \prod_{i=1}^{N_X - N_D} \int_{-\delta/2}^{\delta/2} \sqrt{|\gamma_{\perp_i}|}\, q_Z(z(y))\, \mathrm{d}y_\perp^i\, \mathrm{d}y_\parallel
\end{aligned}
$$

- When $\delta \to 0$, the integration domain shrinks to zero, but the value of the integral is bounded from below

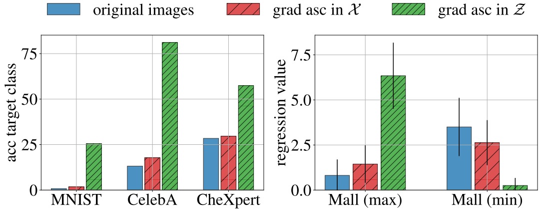
- Hence, the metric $\gamma_{\perp_i}$ has to diverge, i.e. $\gamma_{\perp_i}^{-1} \to 0$.

Eigenvalue spectrum of Jacobian



Quantitative evaluation

- Diffeomorphic Counterfactuals generalize to SVMs, adversarials do not



- The ground truth classes for the ten nearest neighbors matches the target values of the counterfactuals more often for Diffeomorphic Counterfactuals then for adversarials