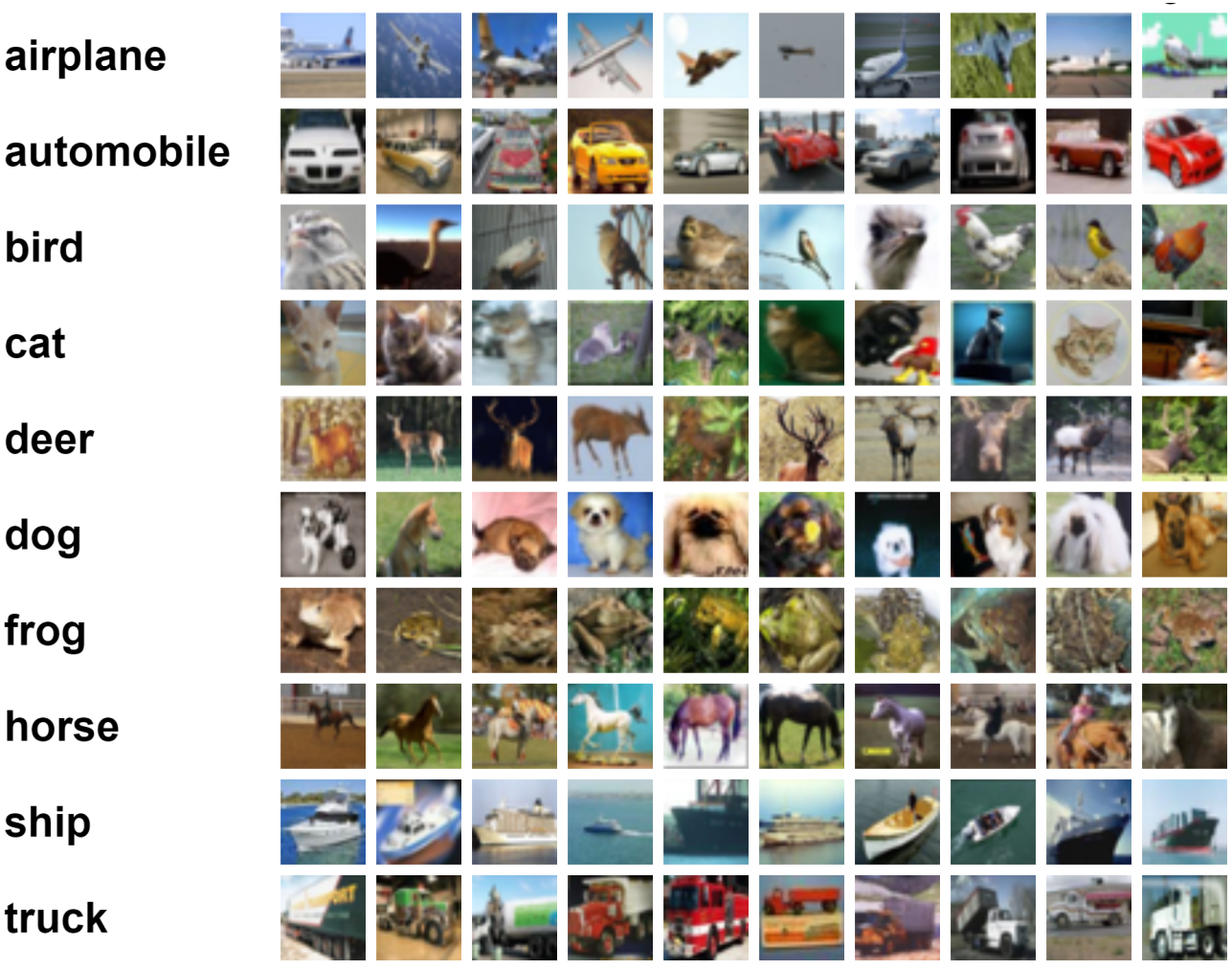
Introduction

Geometry of Data

January 12, 2025

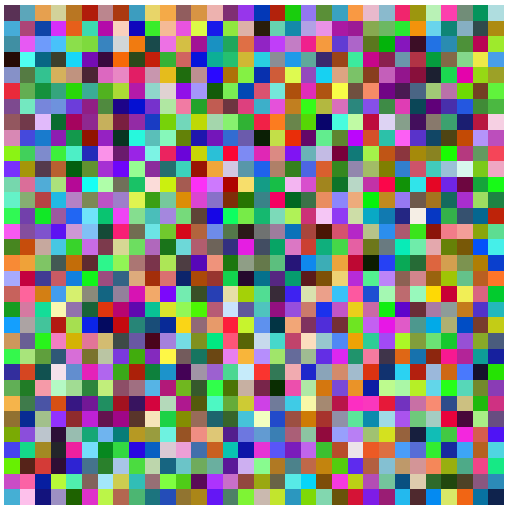
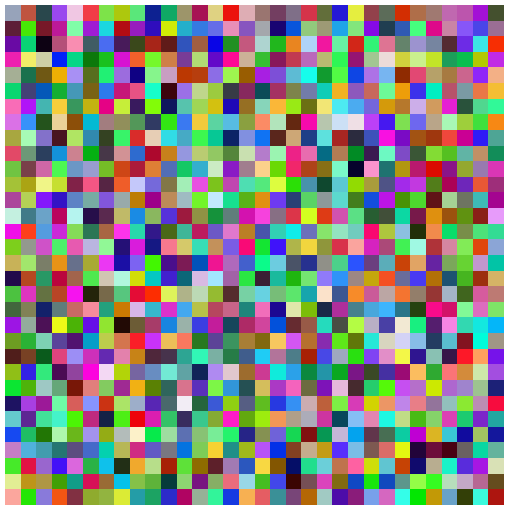
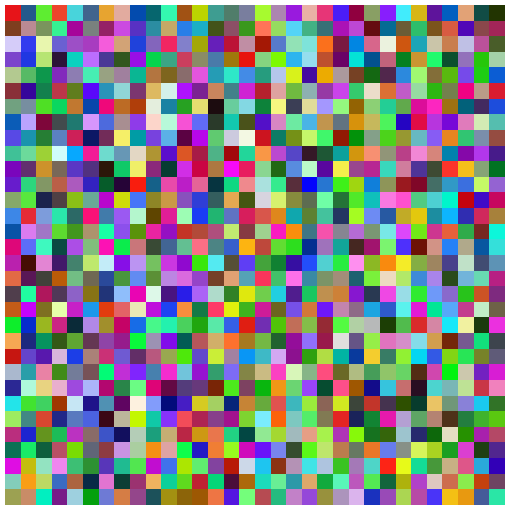
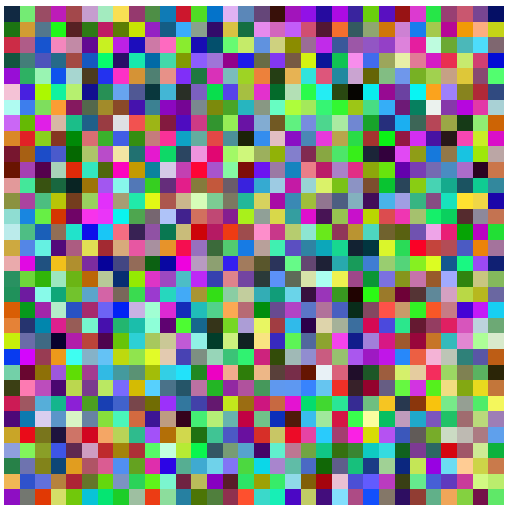
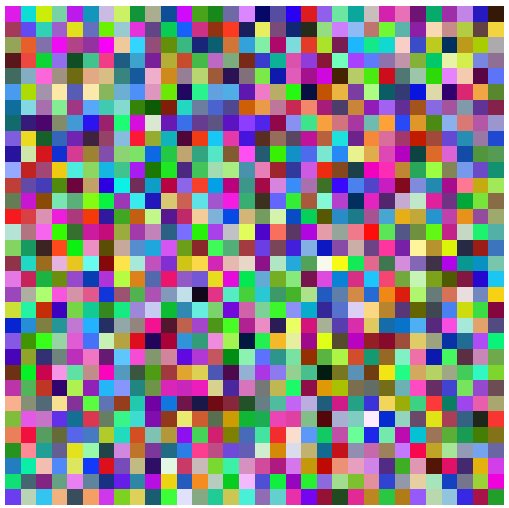
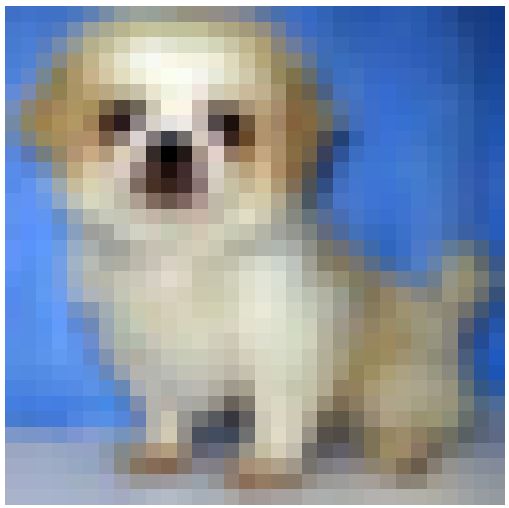
CIFAR-10



$32 \times 32 \times 3 = 3{,}072$ dimensions

10 classes

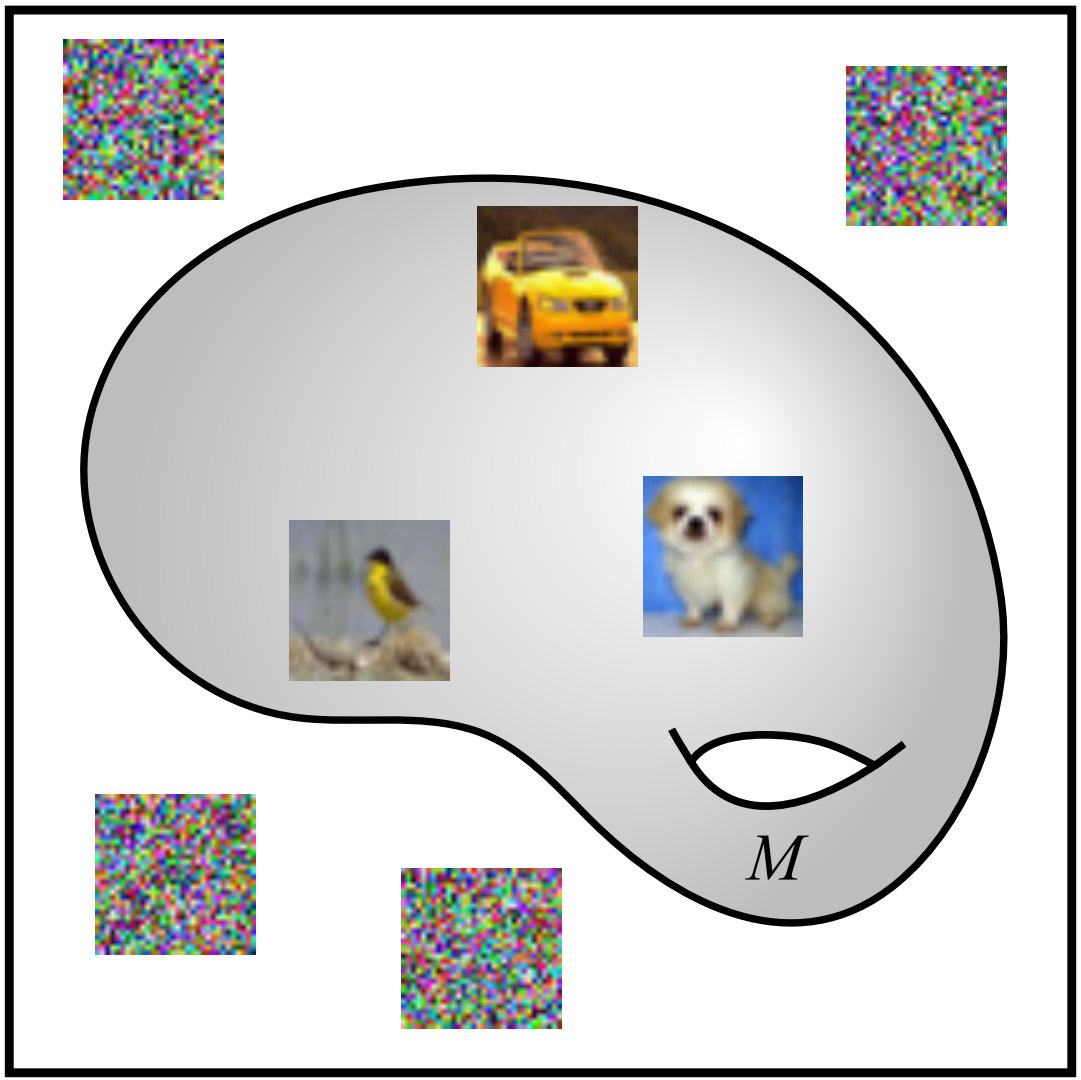
Uniform Random Images

just kidding!

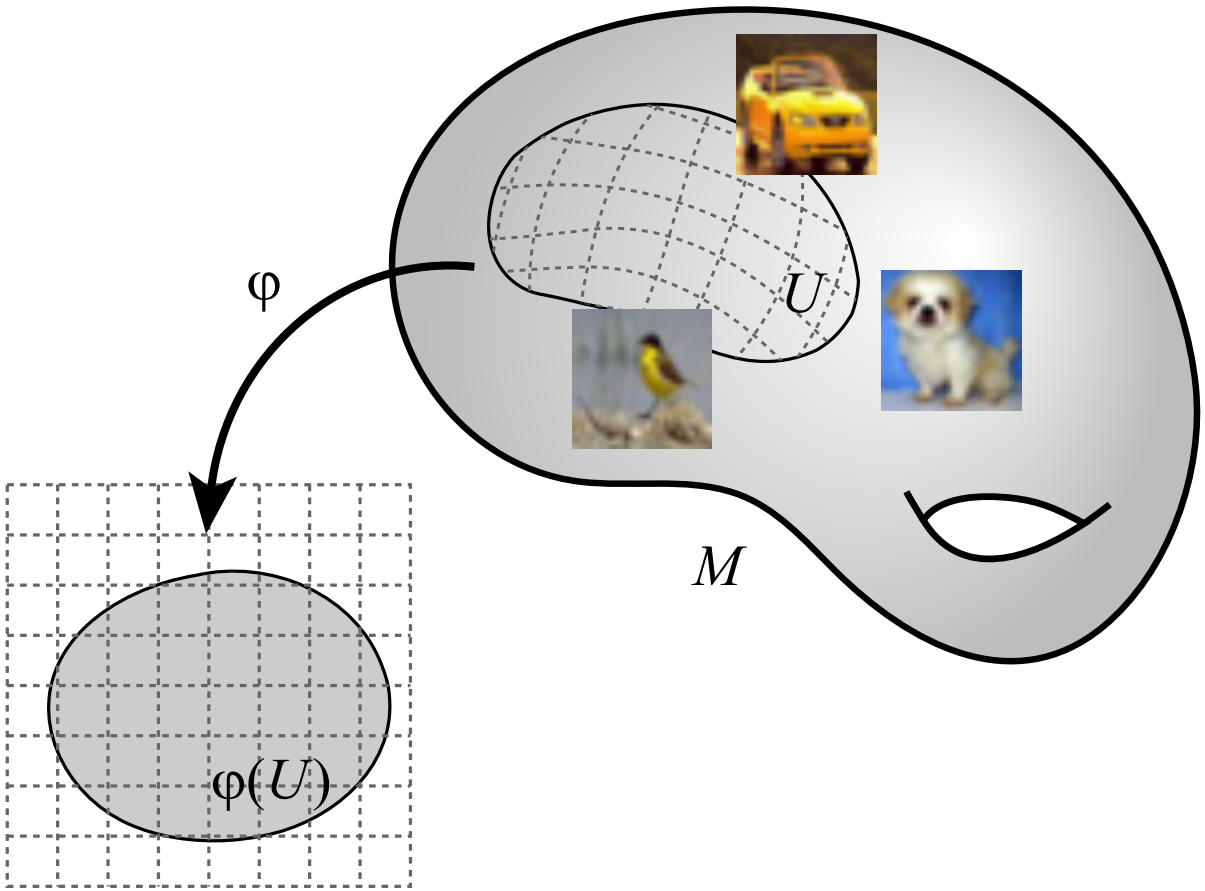
Manifold Hypothesis

Real data lie near lower-dimensional manifolds

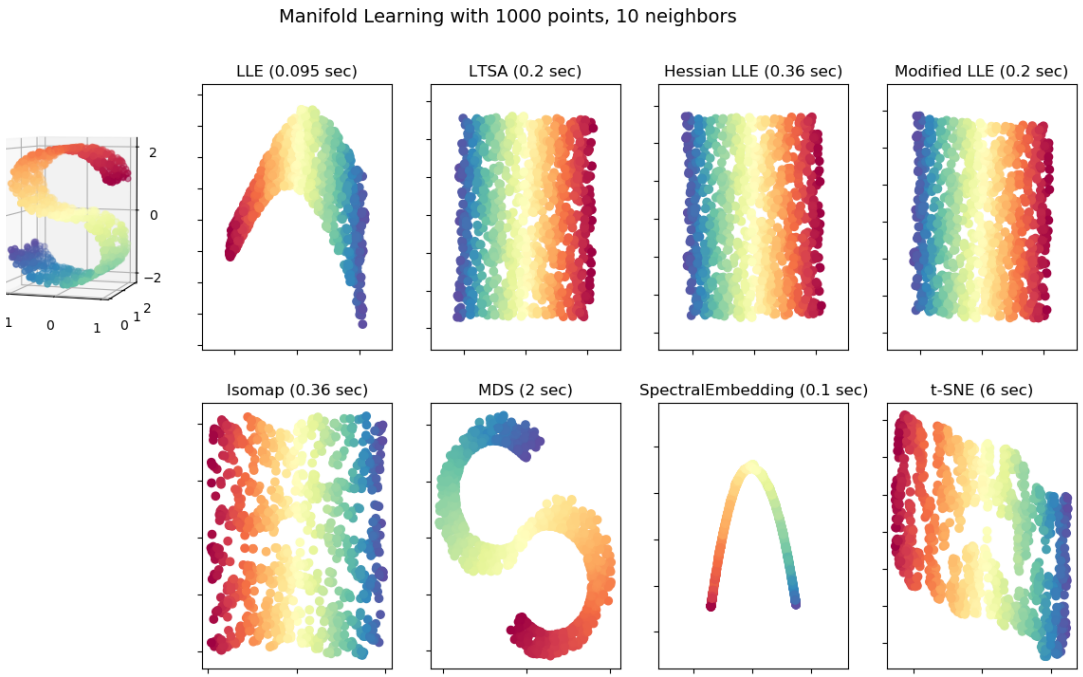


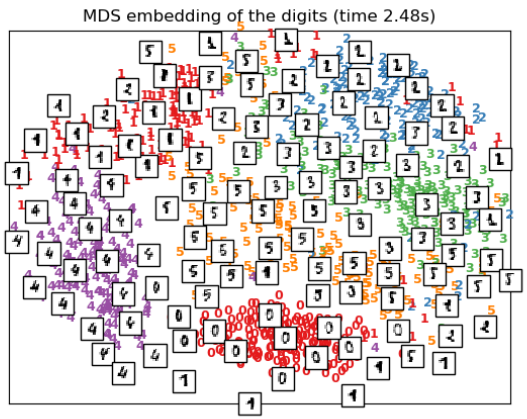
Manifold Learning

- Learn a model/representation for the data manifold
- Often involves finding a flat coordinate chart



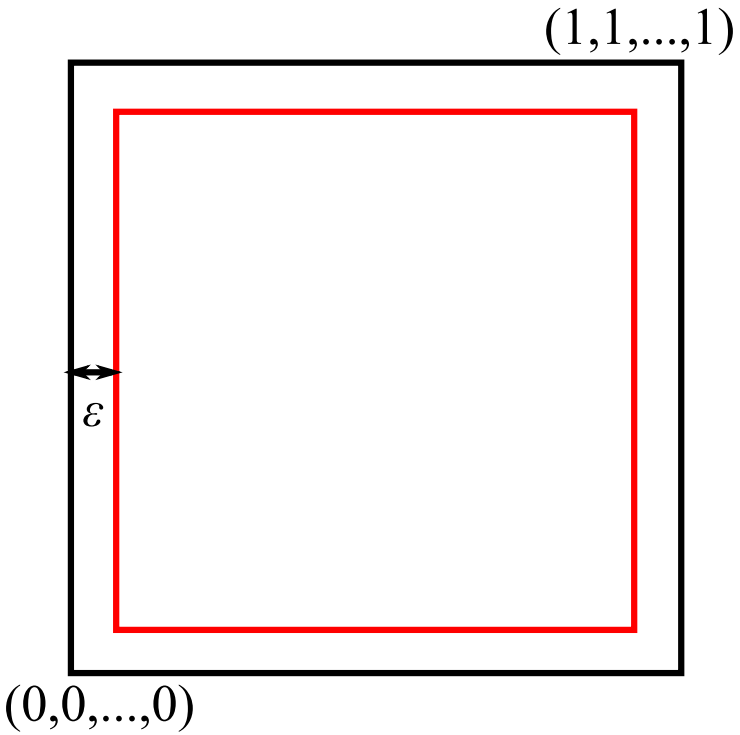
Manifold Learning





From scikit-learn.org

Volumes in High Dimensions



What is the volume of the unit d-cube shrunk by some small amount in each dimension?

$$V = (1 - 2\epsilon)^d$$

Approaches 0 as $d \to \infty$

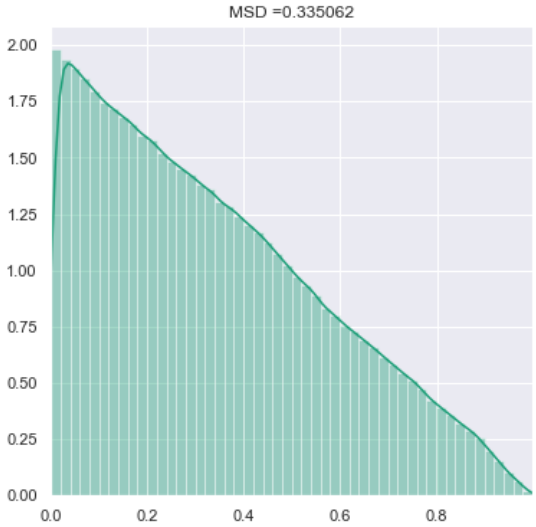
Example: $256 \times 256 \times 3$ images, $\epsilon = \frac{1}{256}$

$$V \approx 2.0 \times 10^{-670}$$

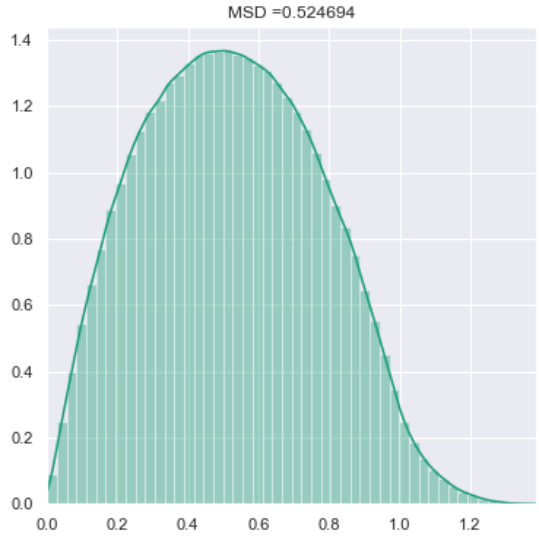
Distances in High Dimensions

Sample two points uniformly from the unit d-cube:
$X, Y \sim \text{Unif}([0,1]^d)$

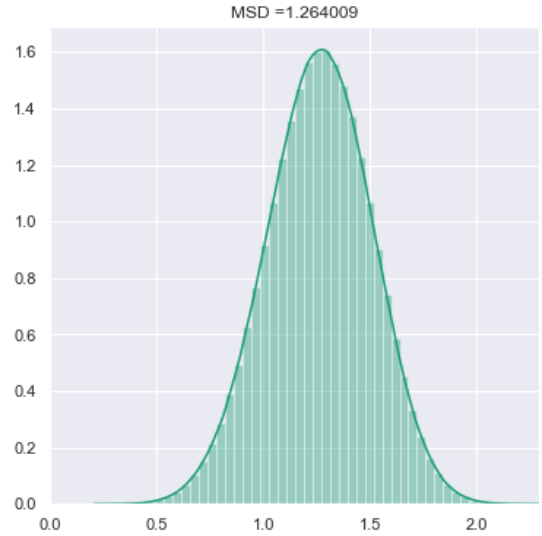
What is the distribution of the distance between them?
$D = \|X - Y\|$



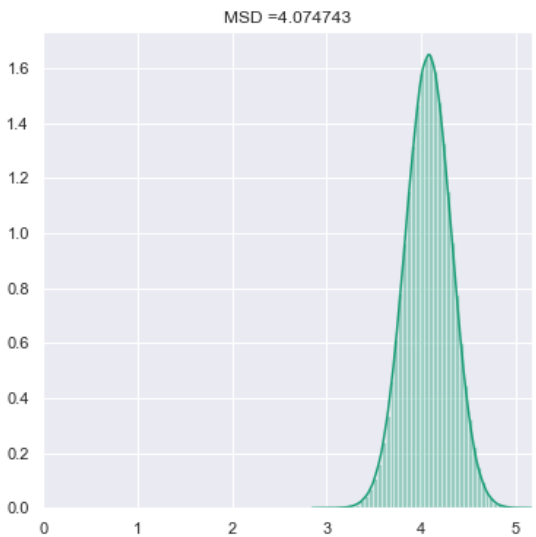
$d = 1$



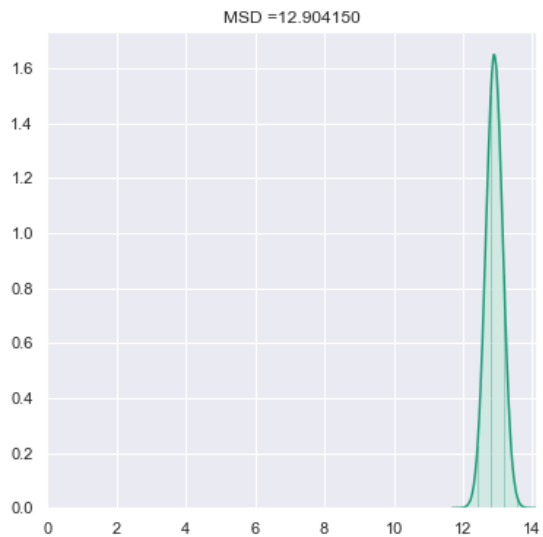
$d = 2$



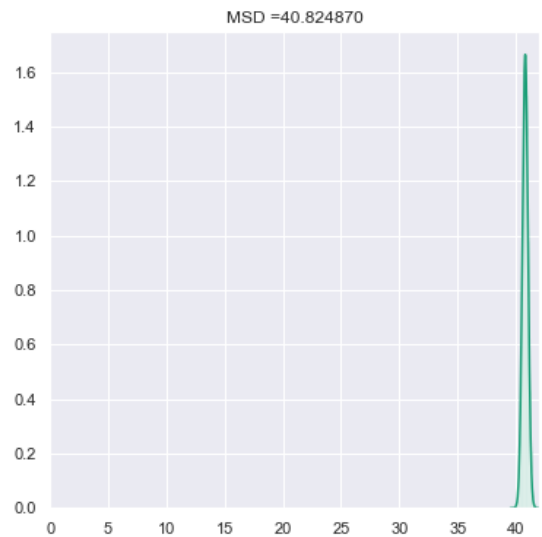
$d = 10$



$d = 100$

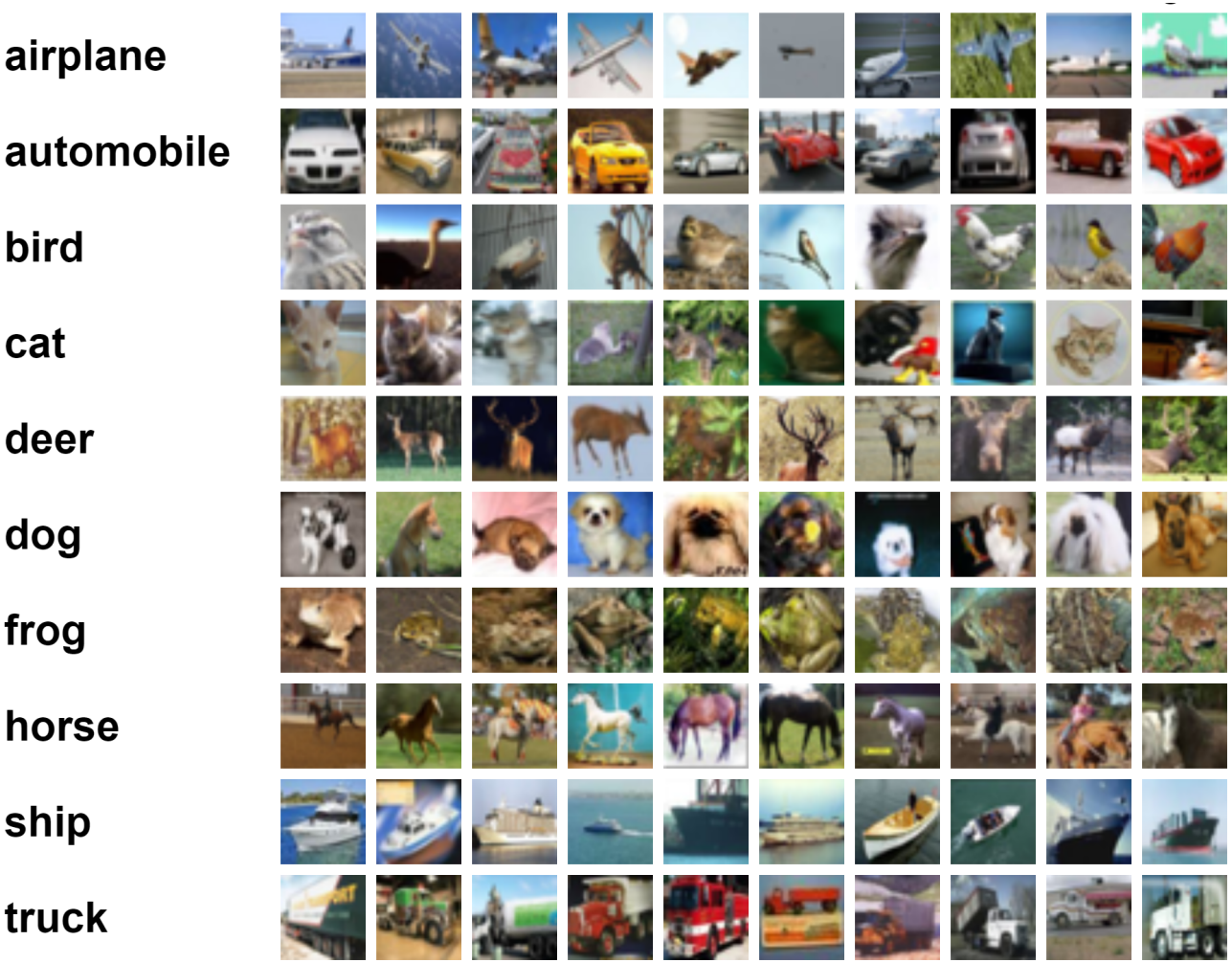


$d = 1{,}000$



$d = 10{,}000$

CIFAR-10



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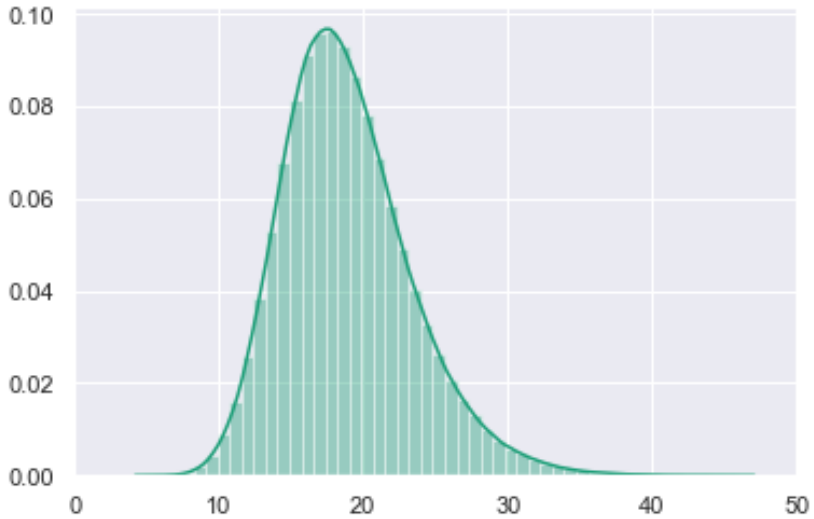
Distances in Real Data



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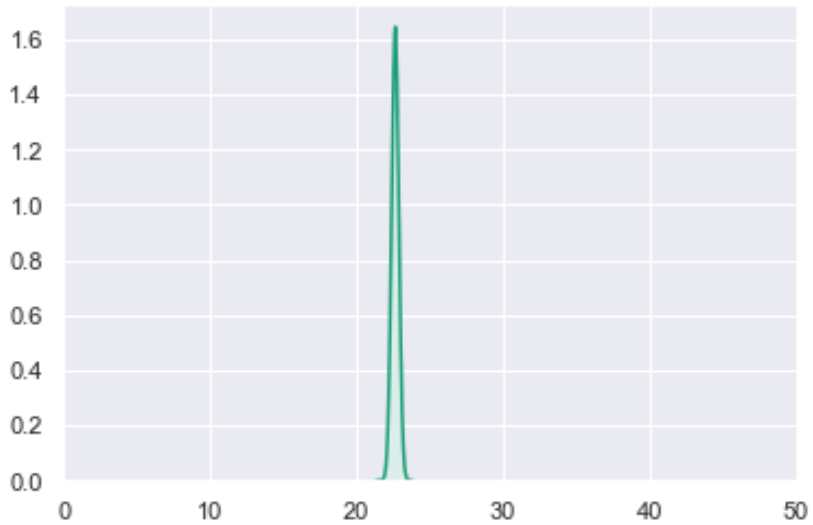


$\text{Unif}([0,1]^{3072})$

Manifold-valued Data

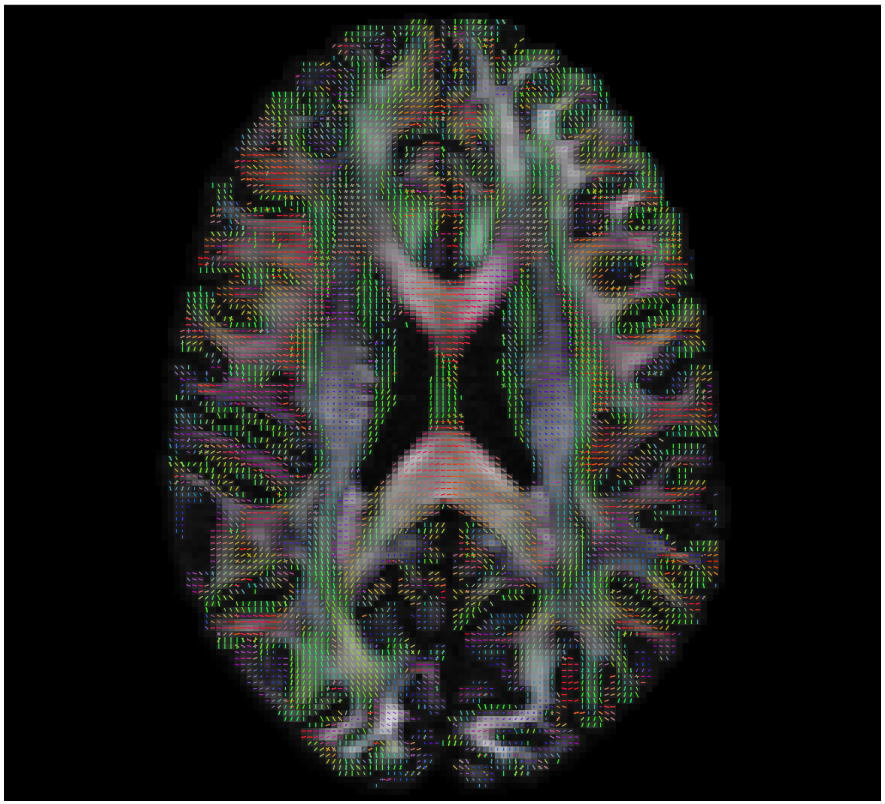
- Manifold already known, not learned
- Manifold arises from natural non-linear constraints on data
- Linear data analyses (in fact, vector space operations) violate these constraints

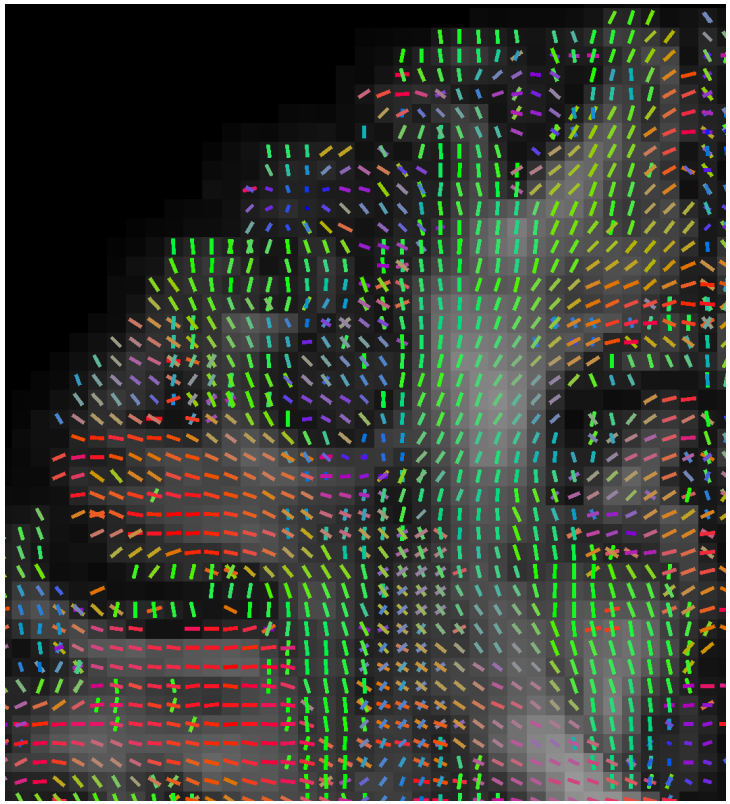
Directional Data

Data living on a circle (S^1) or sphere (S^2), etc.

- Orientation of molecules in protein structure
- Direction of robot or autonomous vehicle
- Position on the earth
- Motion capture: orientation of joints
- Time (time of day, day of the year, etc.)

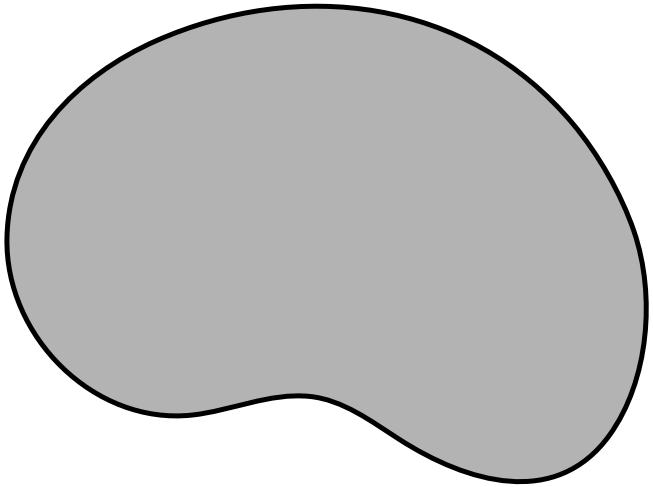
Directional Data: Diffusion MRI





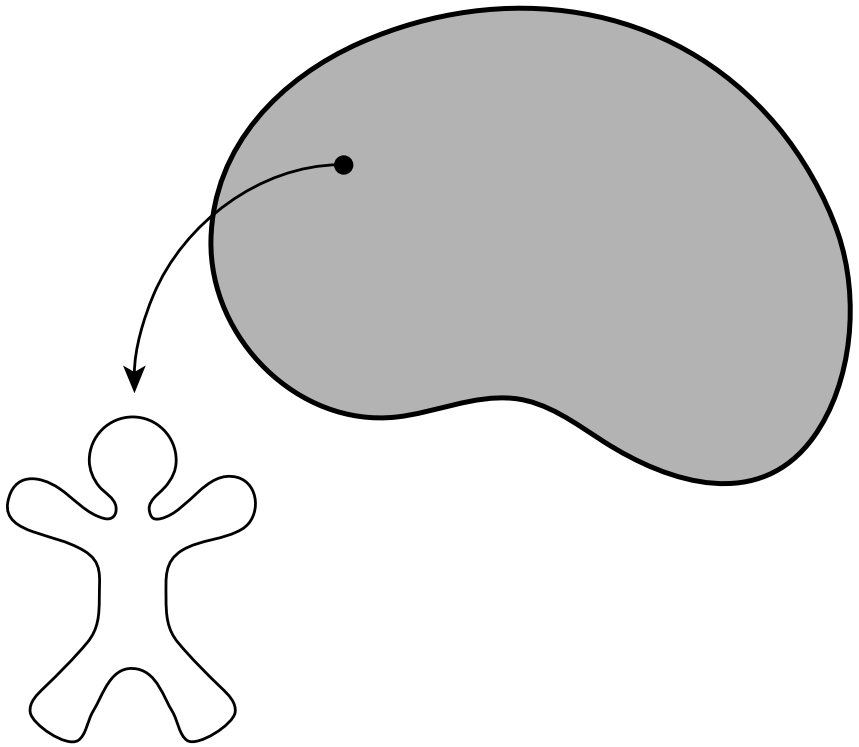
Voxel features are directions of axons in brain

Shape Manifolds



A shape is a point in a high-dimensional, nonlinear manifold, called a **shape space**.

Shape Manifolds



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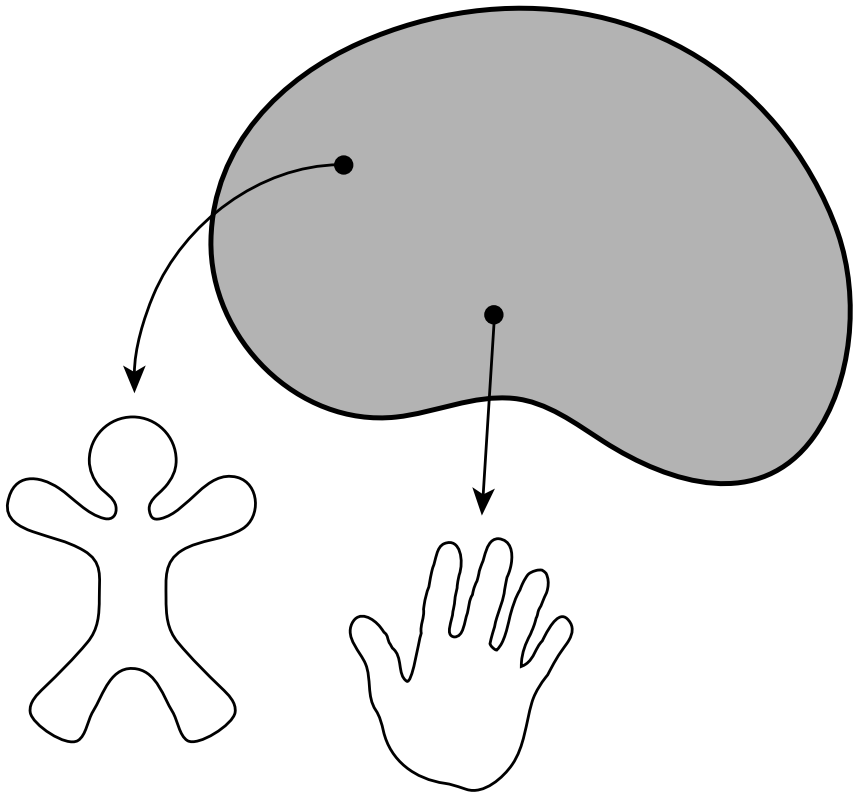

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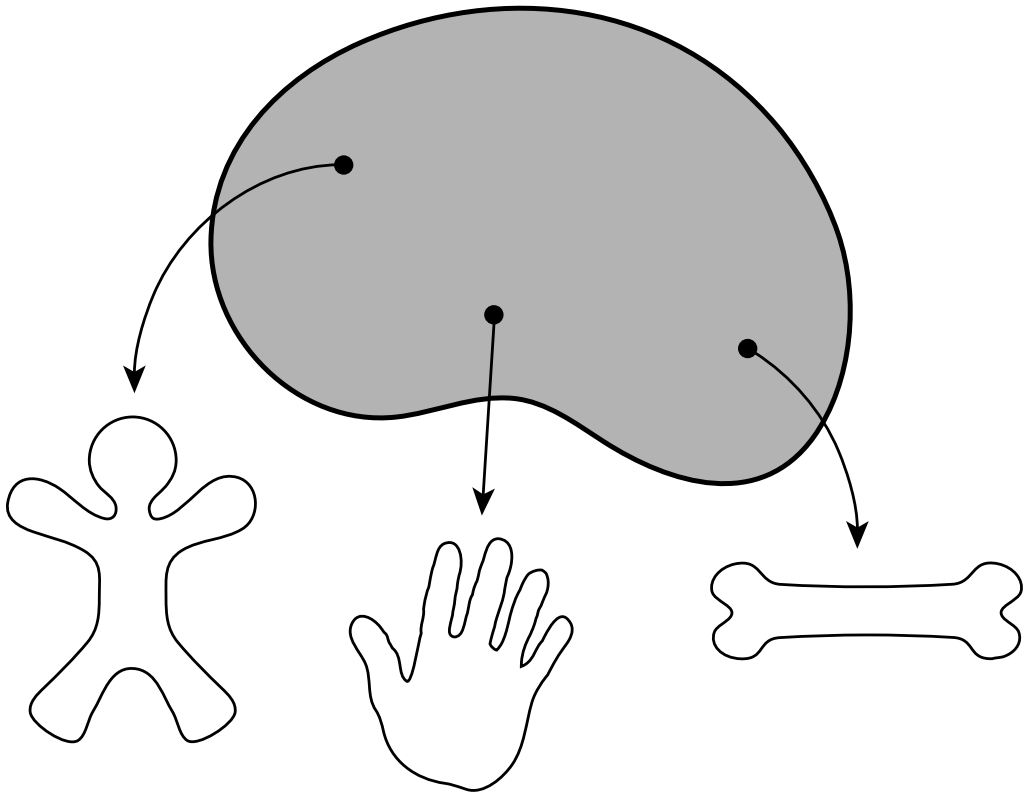

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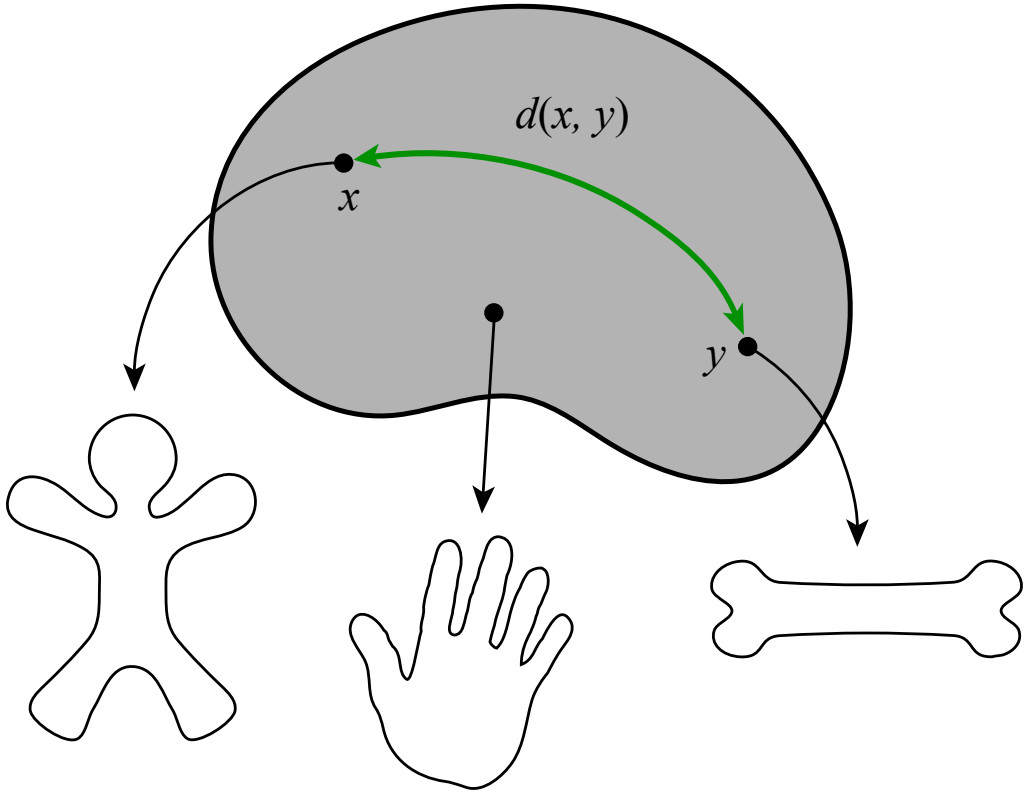
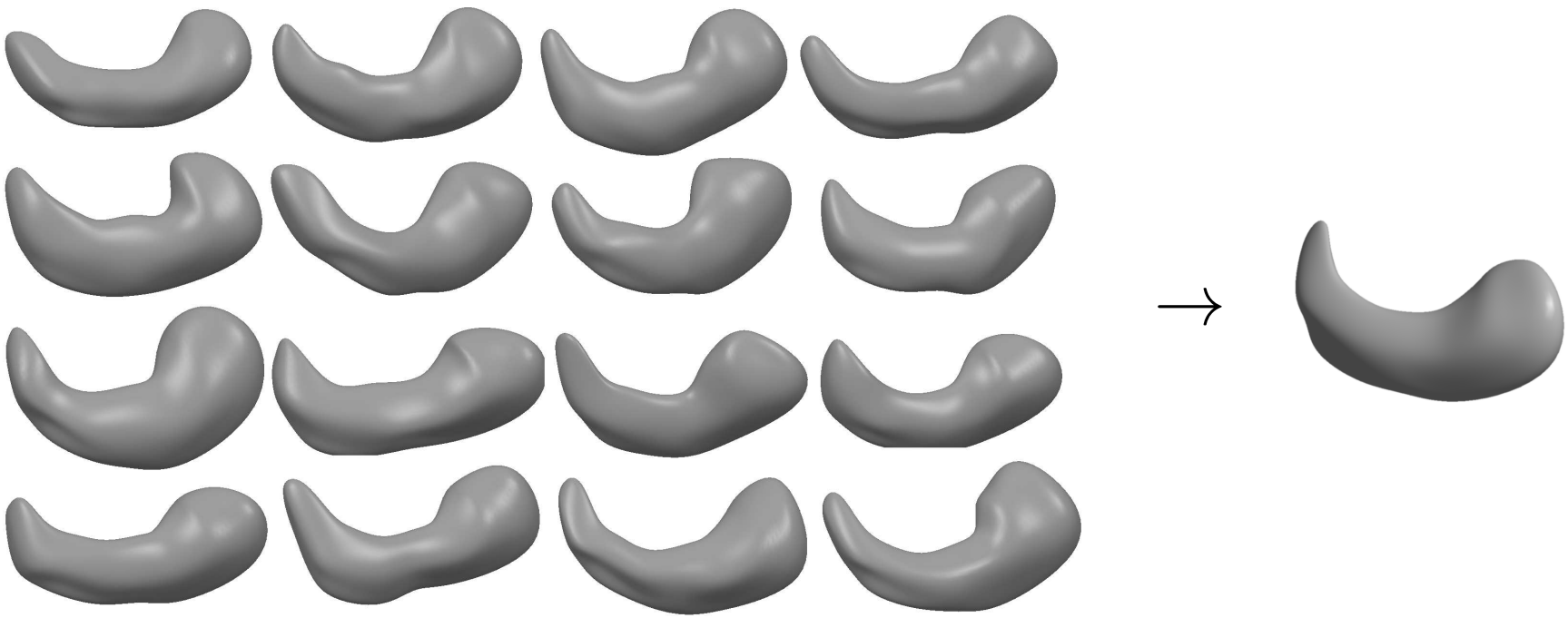
Shape Manifolds

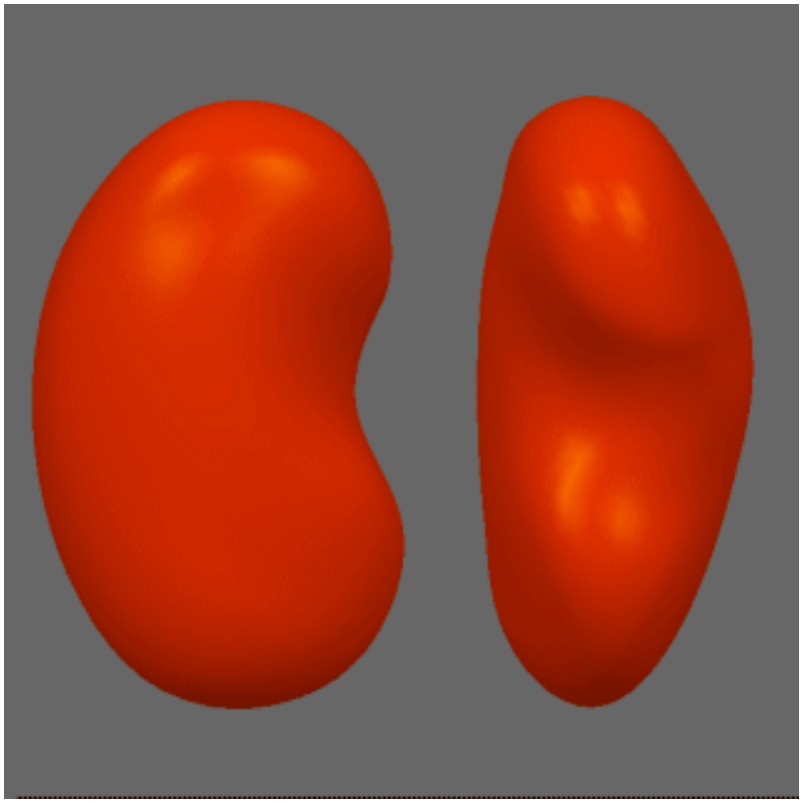


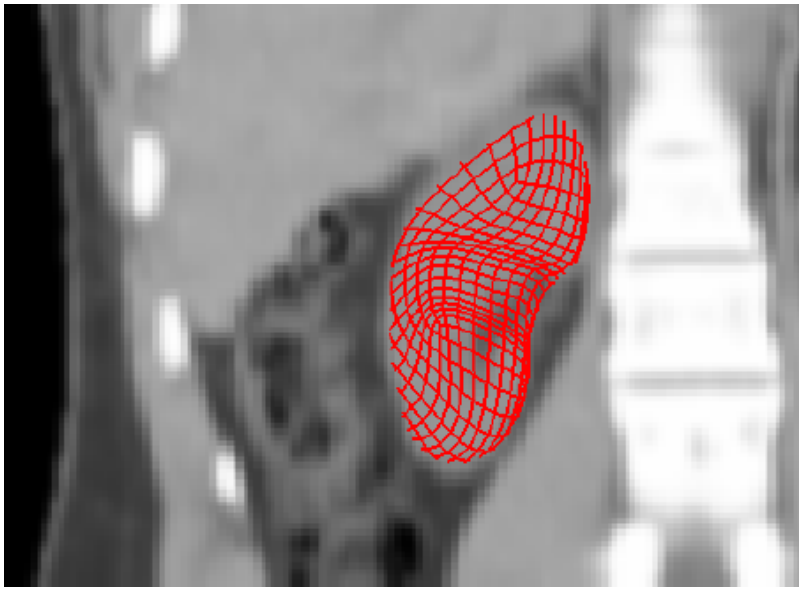
A metric space structure provides a comparison between two shapes.

Shape Statistics: Averages



Shape Statistics: Variability





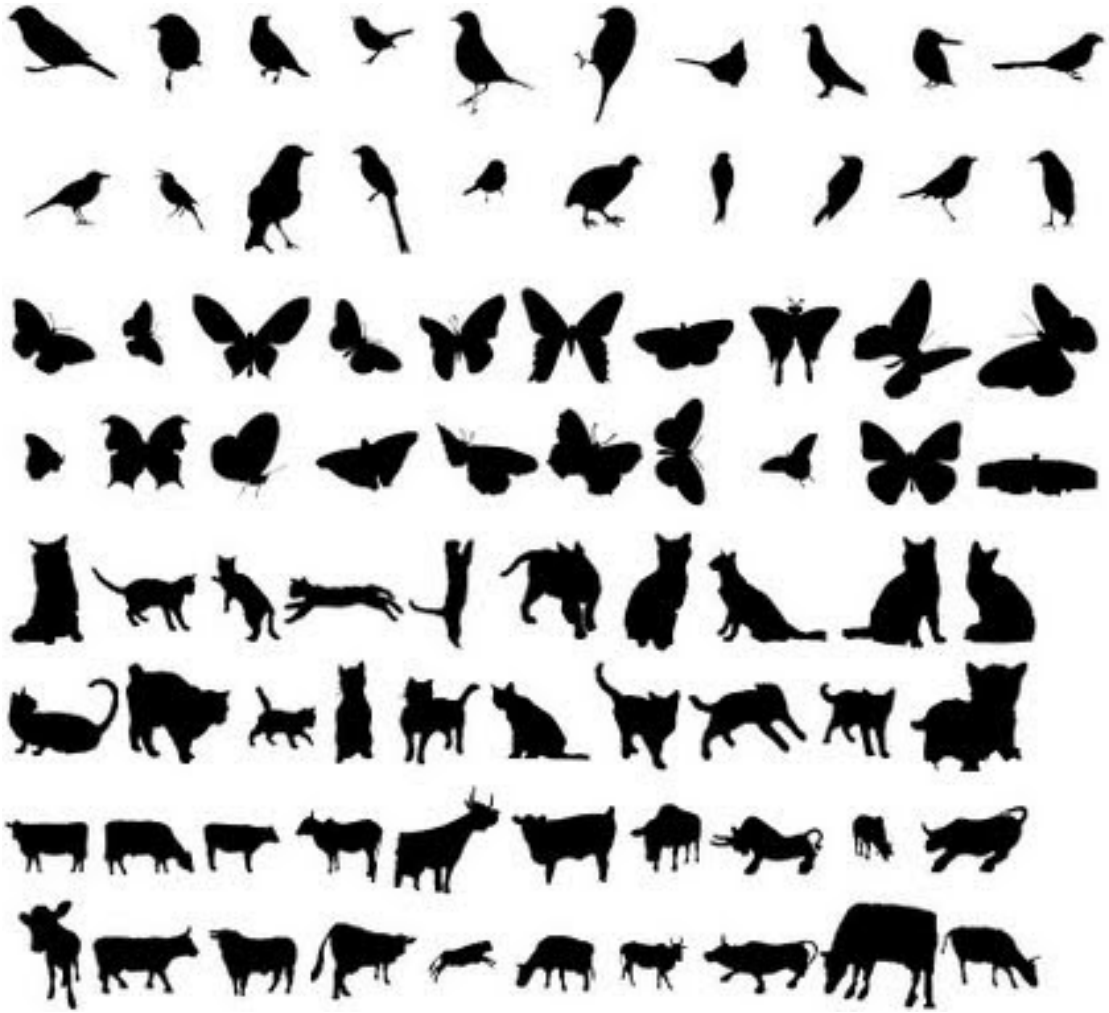
Shape priors in segmentation

Shape Application: Bird Identification

American Crow

Common Raven

Shape Statistics: Classification

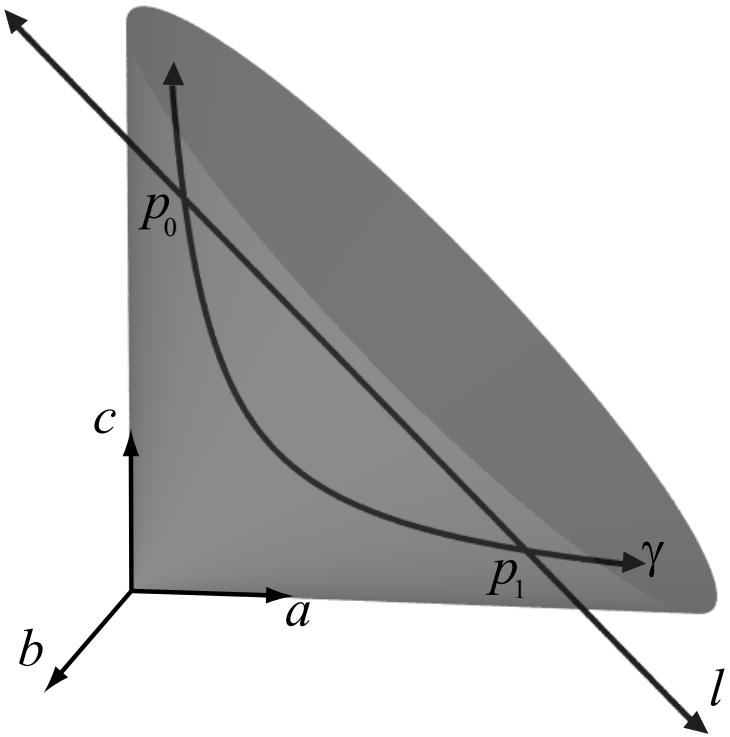


http://sites.google.com/site/xiangbai/animaldataset

Information Geometry

Parameters of a probability model live on manifolds

Example: covariance matrix of a 2D Gaussian distribution:



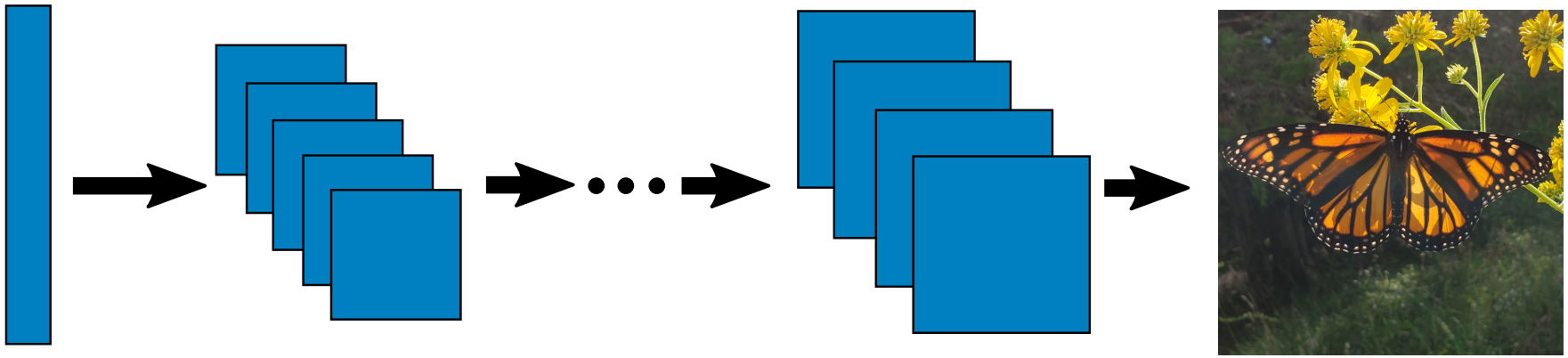
$\Sigma \in \mathrm{PD}(2)$ is of the form

$$\Sigma = \begin{pmatrix} a & b \\ b & c \end{pmatrix},$$

$$ac - b^2 > 0, \quad a > 0.$$

(positive-definite constraint)

Deep Generative Models



Input:

$z \in \mathbb{R}^d$

$z \sim N(0, I)$

$\xrightarrow{g = g_L \circ g_{L-1} \circ \cdots \circ g_1}$

Output:

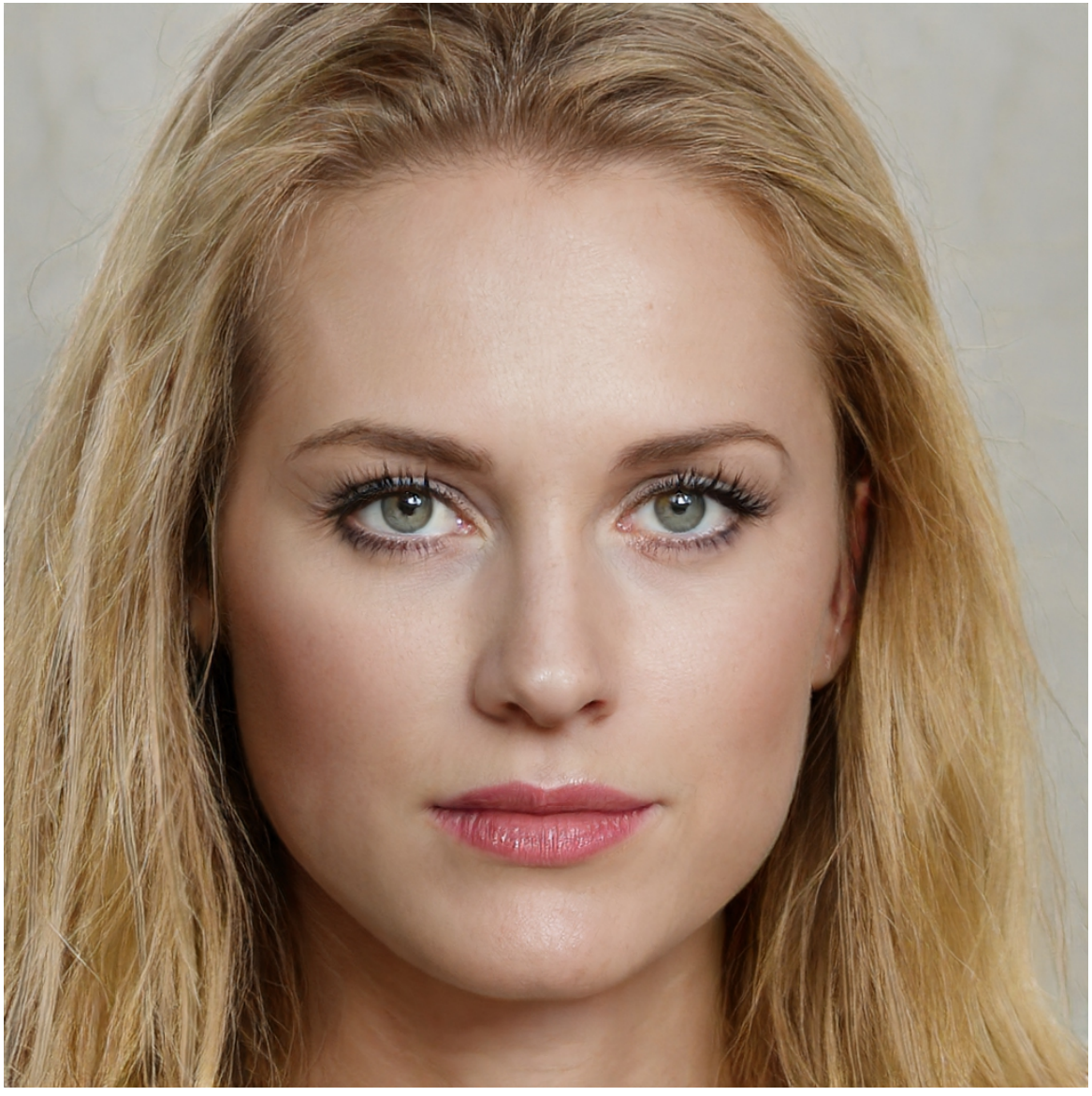
$x \in \mathbb{R}^D$

$d << D$

These are not real people

Karras et al., CVPR 2020, and thispersondoesnotexist.com

These are not real people



Karras et al., CVPR 2020, and thispersondoesnotexist.com

These are not real people

Karras et al., CVPR 2020, and thispersondoesnotexist.com

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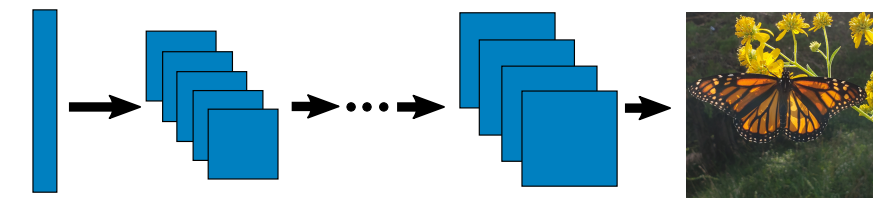
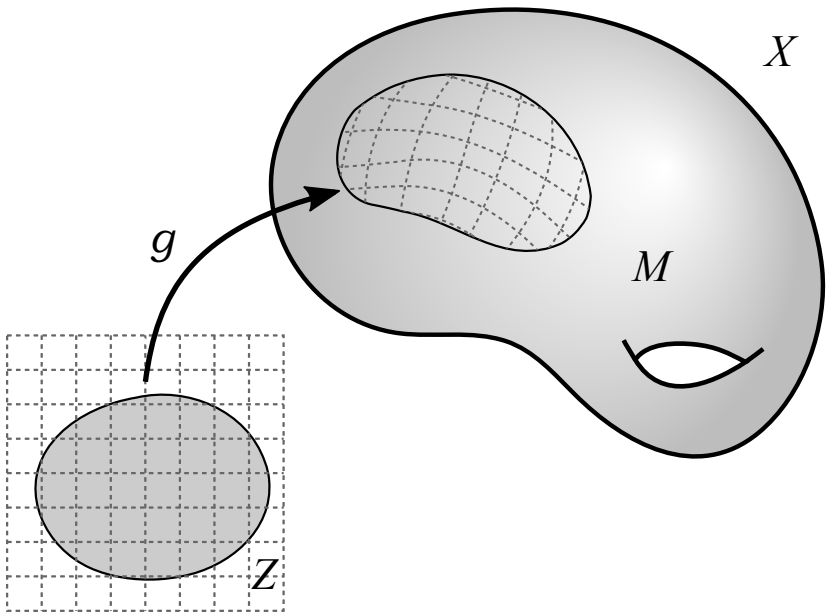
Generative Models as Immersed Manifolds



$z \in \mathbb{R}^d \xrightarrow{g = g_L \circ g_{L-1} \circ \cdots \circ g_1} x \in \mathbb{R}^D$



Shao, Kumar, Fletcher, The Riemannian Geometry of Deep Generative Models, DiffCVML 2018.