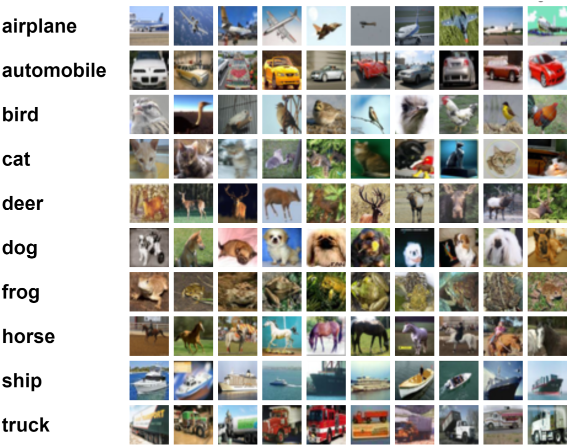
Introduction

Geometry of Data

August 27, 2024

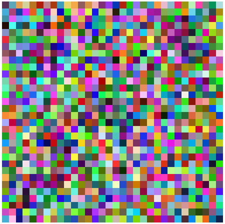
CIFAR-10



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

10 classes

Uniform Random Images



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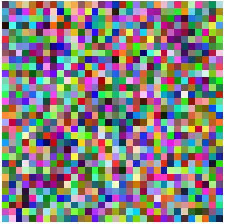

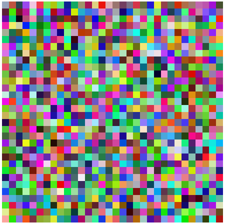

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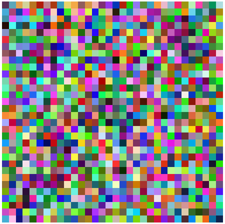
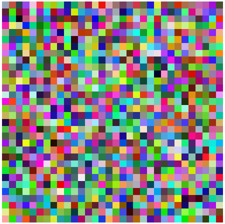
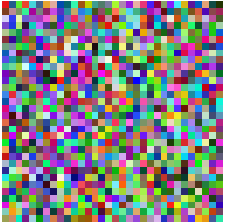

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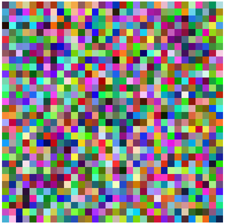
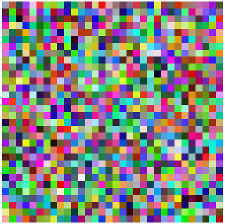
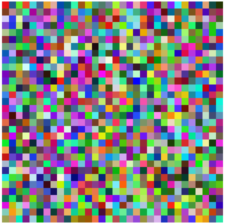
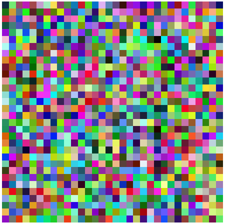

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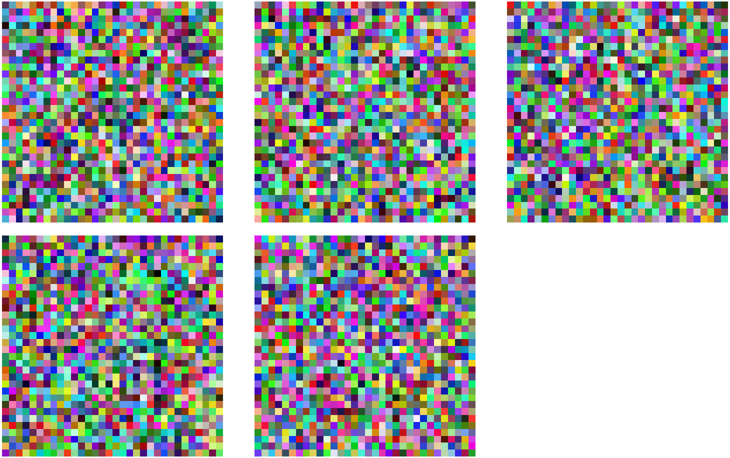

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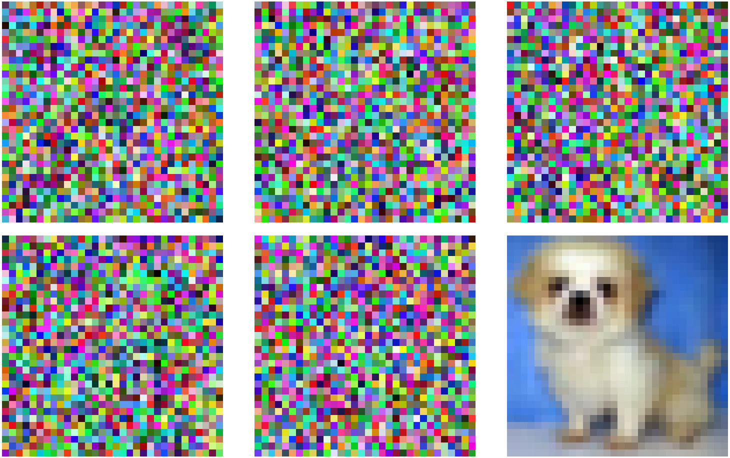

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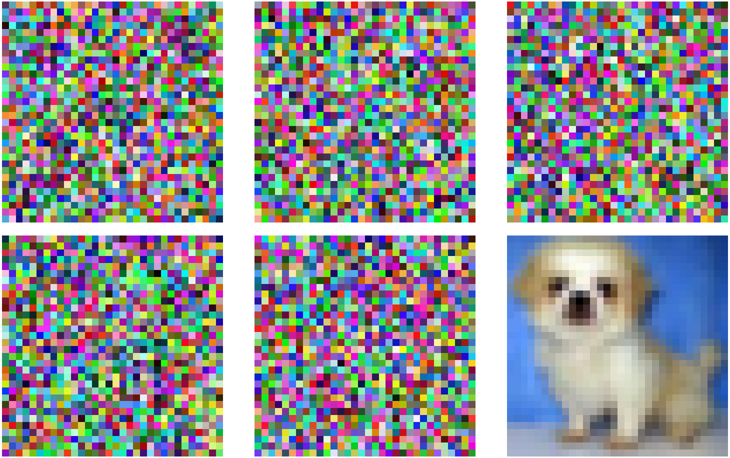
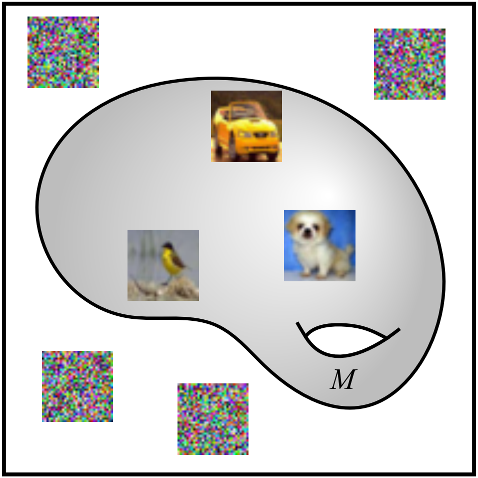


just kidding!

Manifold Hypothesis

Real data lie near lower-dimensional manifolds



Manifold Learning

Manifold Learning

- Learn a model/representation for the data manifold

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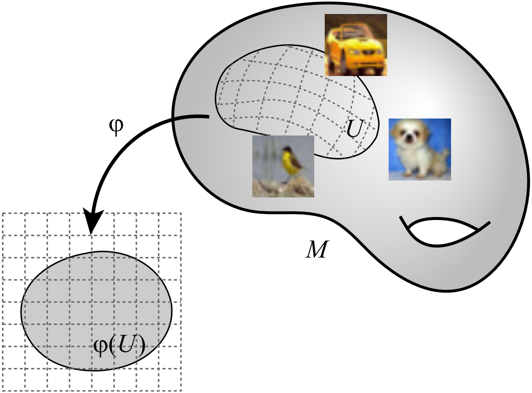

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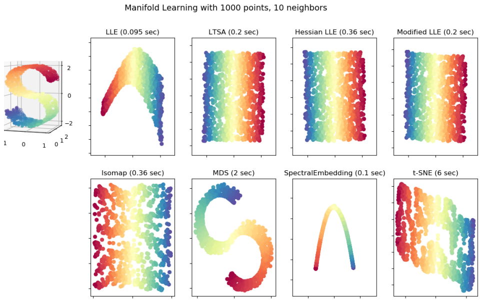
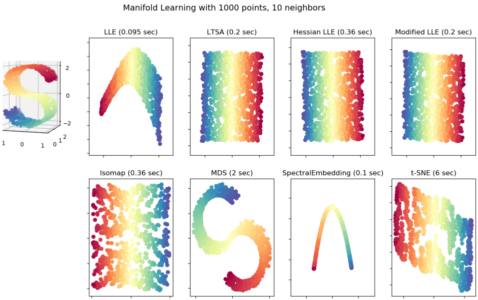
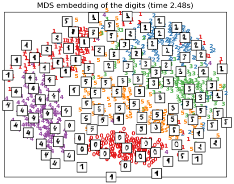


From scikit-learn.org

Manifold Learning





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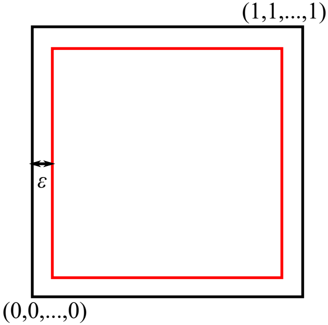
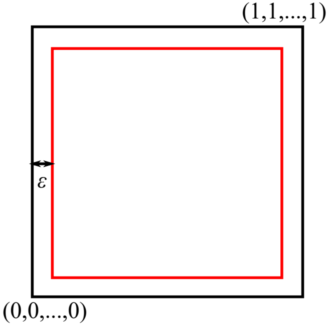
Volumes in High Dimensions



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

Volumes in High Dimensions



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

Approaches 0 as $d \to \infty$

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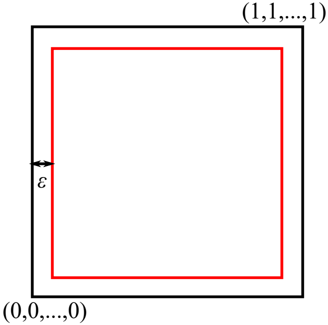

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Example: $256 \times 256 \times 3$ images, $\epsilon = \frac{1}{256}$

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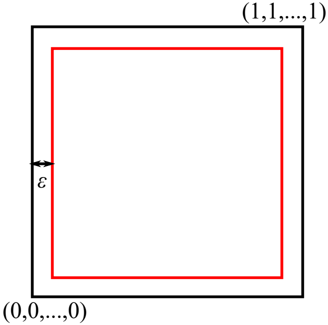

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$$V = (1 - 2\epsilon)^d$$

Approaches 0 as $d \to \infty$

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

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

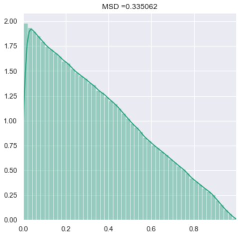
Distances in High Dimensions

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

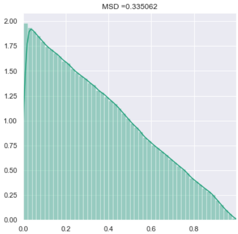
Distances in High Dimensions

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

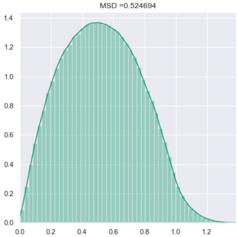
What is the distribution of the distance between them?
$D = \|X - Y\|$



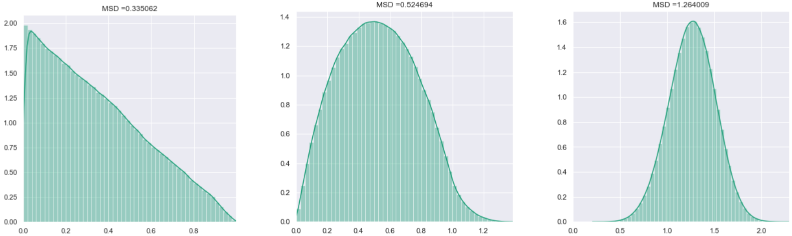
$d = 1$


MSD =0.335062
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
0.0
0.2
0.4
0.6
0.8

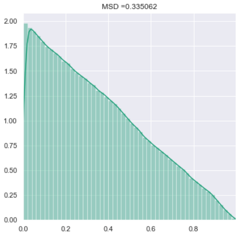
$d = 1$


MSD =0.524694
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
1.2

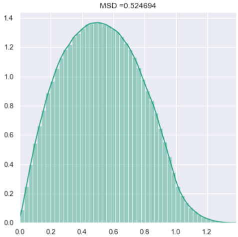
$d = 2$



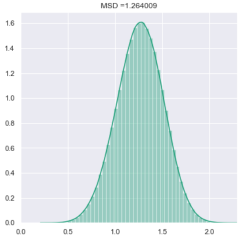
$d = 1$ $\quad$ $d = 2$ $\quad$ $d = 10$



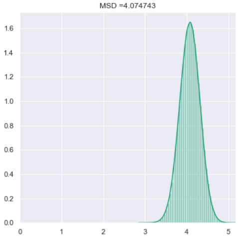
$d = 1$



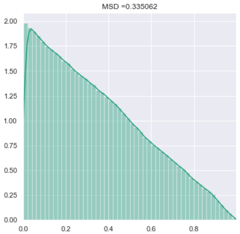
$d = 2$



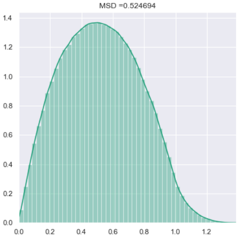
$d = 10$



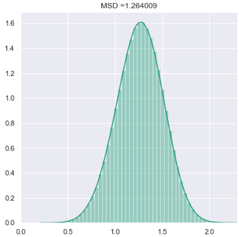
$d = 100$



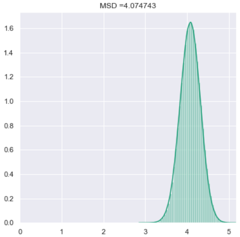
$d = 1$



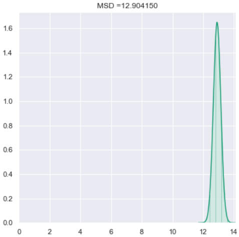
$d = 2$



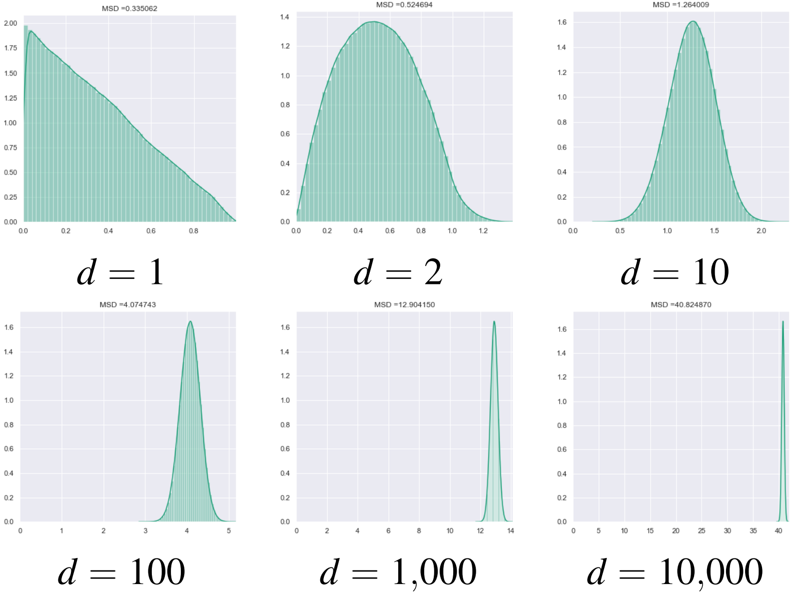
$d = 10$



$d = 100$

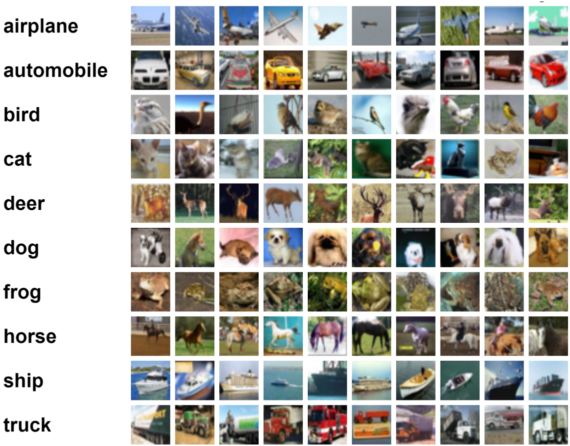


$d = 1{,}000$



MSD =0.335062
MSD =0.524694
MSD =1.264009
$d = 1$
$d = 2$
$d = 10$
MSD =4.074743
MSD =12.904150
MSD =40.824870
$d = 100$
$d = 1,000$
$d = 10,000$

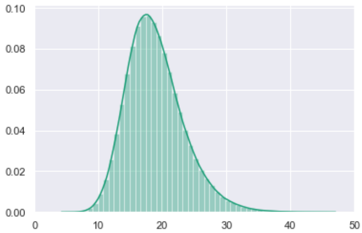
CIFAR-10



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

10 classes

Distances in Real Data



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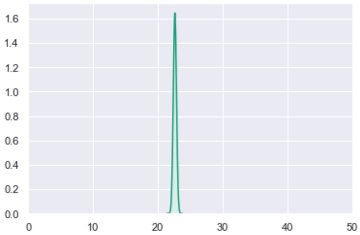

$\mathrm{Unif}([0,1]^{3072})$

Manifold-valued Data

- Manifold already known, not learned

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- Manifold arises from natural non-linear constraints on data

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.

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- Orientation of molecules in protein structure

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- Direction of robot or autonomous vehicle

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- Motion capture: orientation of joints

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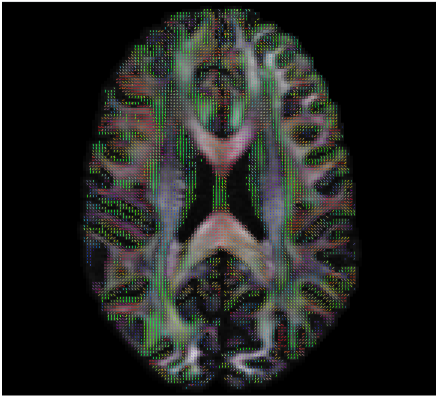
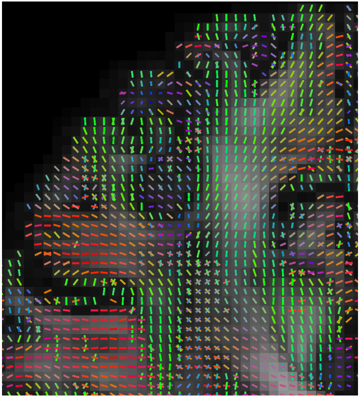
- Motion capture: orientation of joints
- Time (time of day, day of the year, etc.)

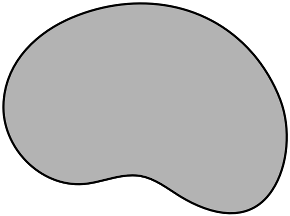
Directional Data: Diffusion MRI





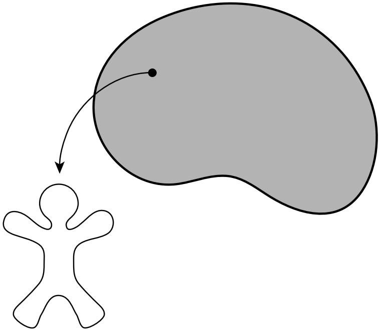
Voxel features are directions of axons in brain

Shape Manifolds



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

Shape Manifolds



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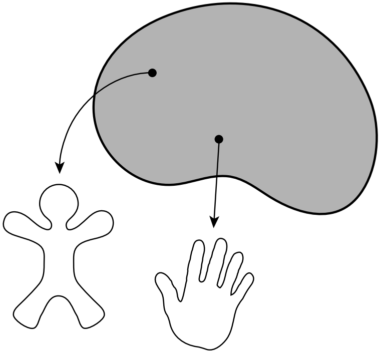

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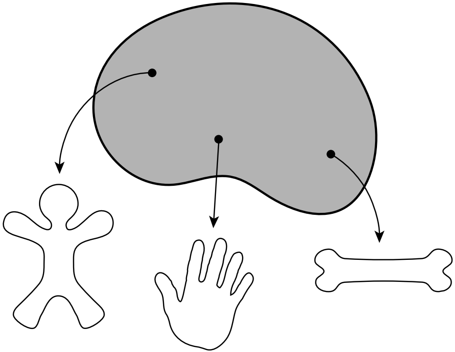

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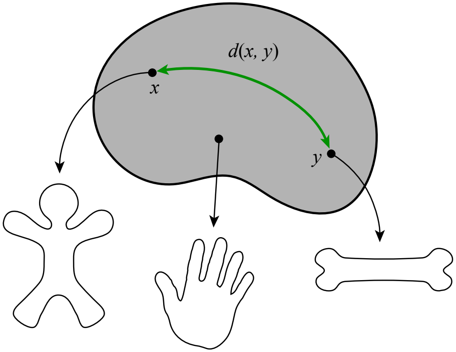
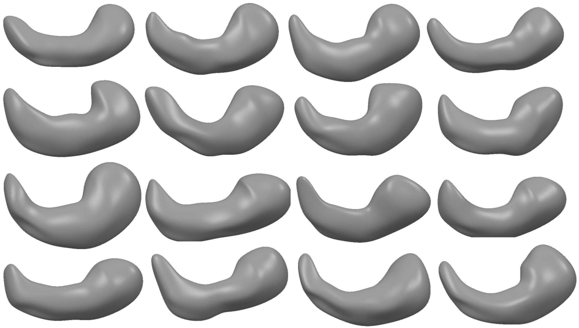


A metric space structure provides a comparison between two shapes.

Shape Statistics: Averages



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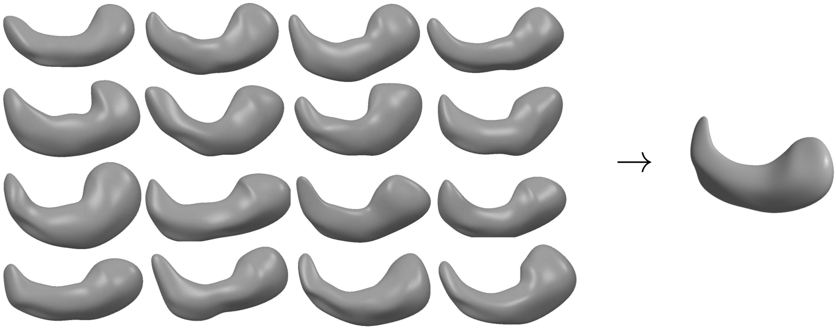
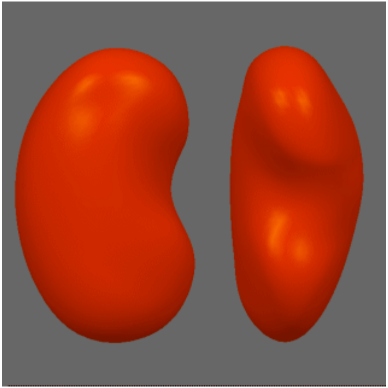
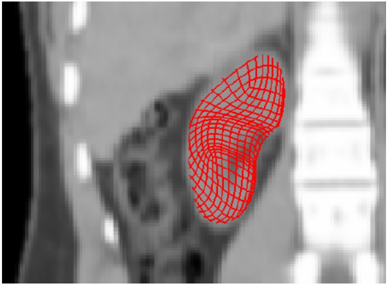


Shape Statistics: Variability





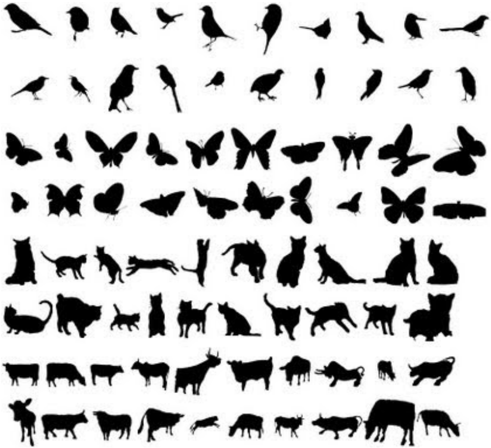
Shape priors in segmentation

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

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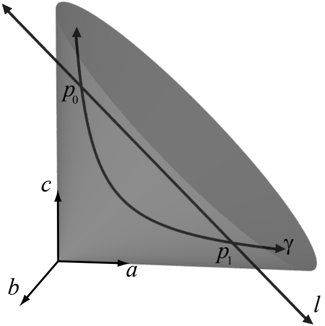
Parameters of a probability model live on manifolds

Example: covariance matrix of a 2D Gaussian distribution:



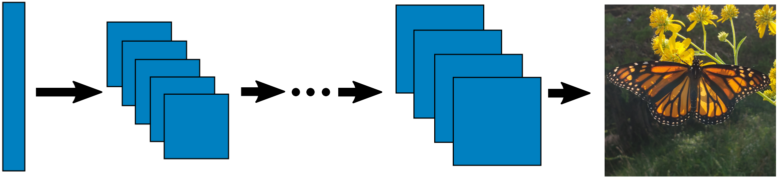
$\Sigma \in \mathrm{PD}(2)$ is of the form

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

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

(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:

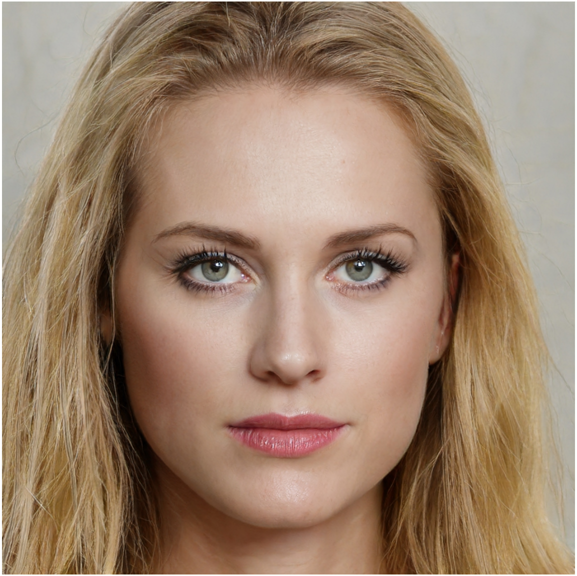
$x \in \mathbb{R}^D$

$$d << D$$

These are not real people

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

These are not real people



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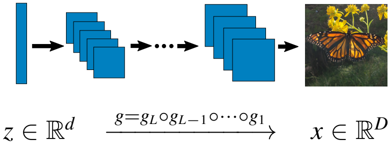
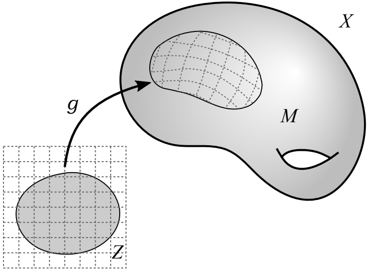
Generative Models as Immersed Manifolds





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