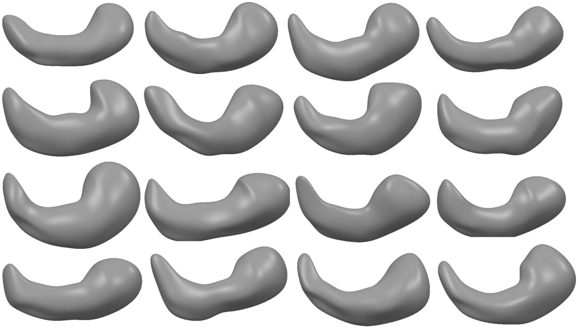
# Introduction to Shape Manifolds

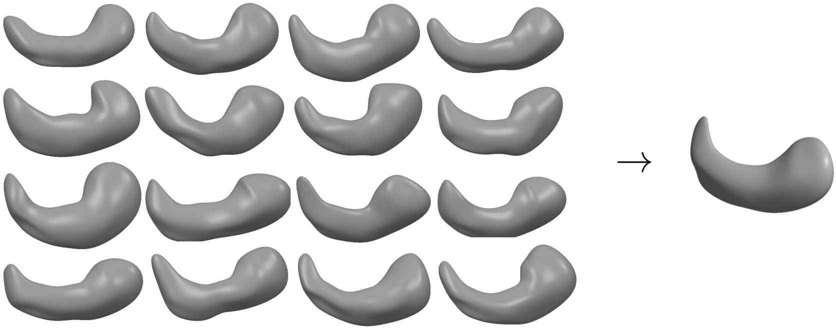
Geometry of Data

September 26, 2019

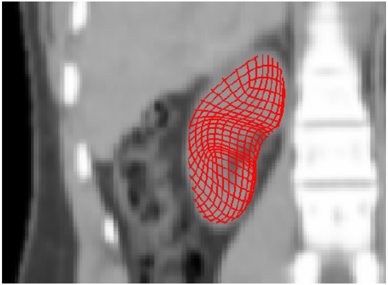
# Shape Statistics: Averages



# Shape Statistics: Averages

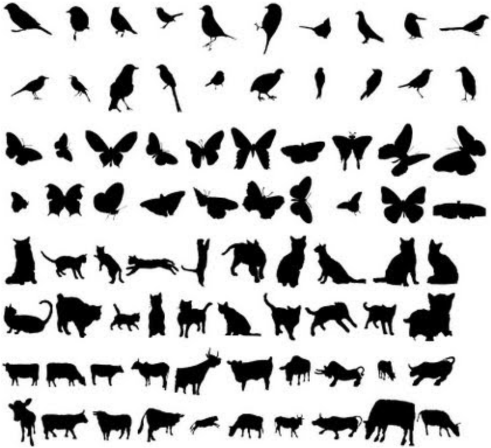


# Shape Statistics: Variability



Shape priors in segmentation

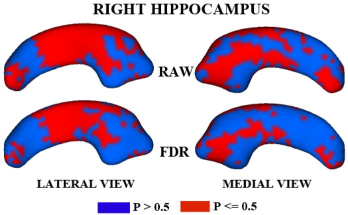
# Shape Statistics: Classification

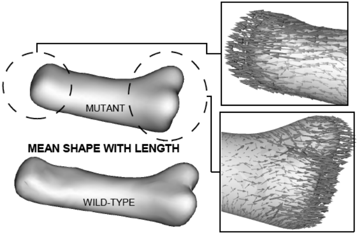


http://sites.google.com/site/xiangbai/animaldataset

# Shape Statistics: Hypothesis Testing

Testing group differences




Cates, et al. IPMI 2007 and ISBI 2008

# Shape Application: Bird Identification

American Crow


Common Raven

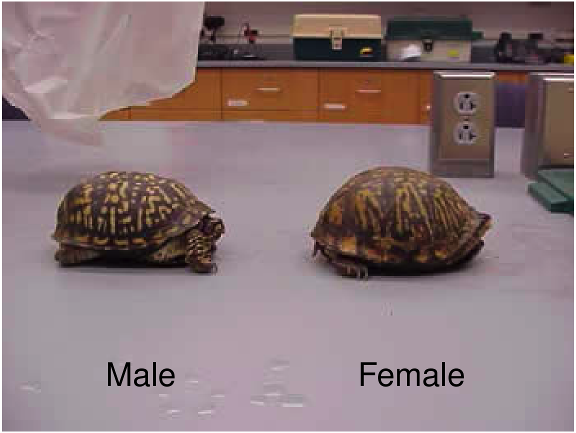
# Shape Application: Bird Identification

Glaucous Gull


Iceland Gull

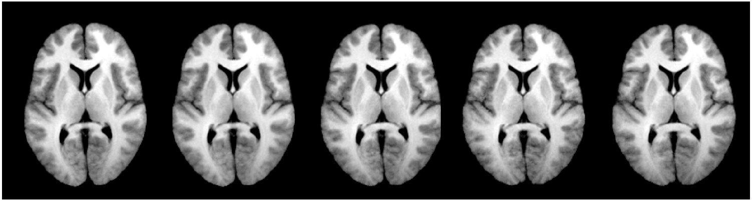

http://notendur.hi.is/yannk/specialities.htm

# Shape Application: Box Turtles

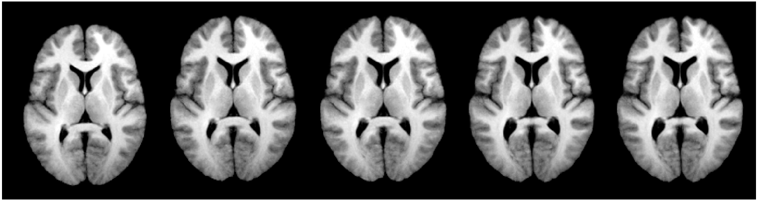



http://www.bio.davidson.edu/people/midorcas/research/Contribute/boxturtle/boxinfo.htm

# Shape Statistics: Regression

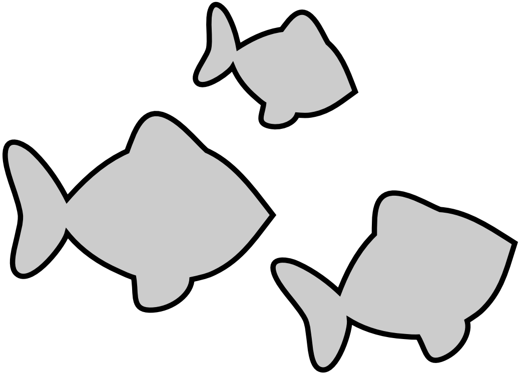


35 37 39 41 43

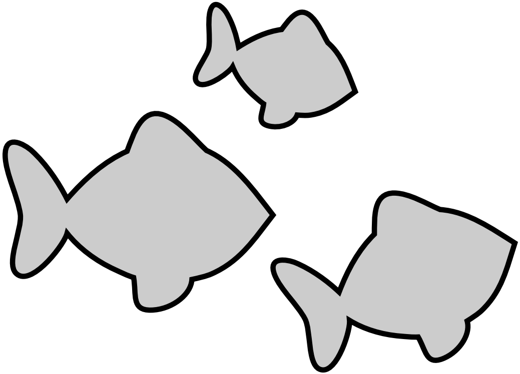


45 47 49 51 53

# What is Shape?



# What is Shape?

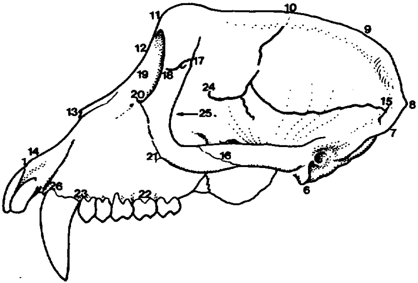


Shape is the geometry of an object modulo position, orientation, and size.

# Geometry Representations

- Landmarks (key identifiable points)
- Boundary models (points, curves, surfaces, level sets)
- Interior models (medial, solid mesh)
- Transformation models (splines, diffeomorphisms)

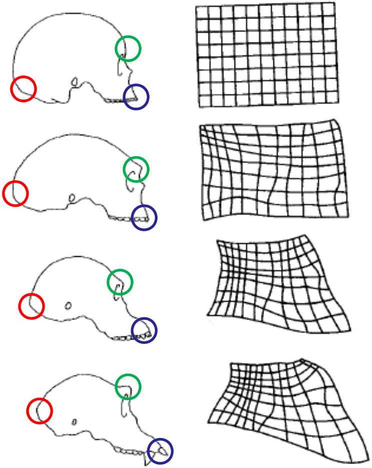
# Landmarks




From Dryden & Mardia, 1998

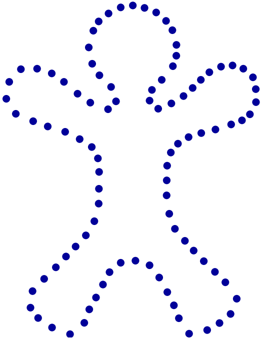
- A **landmark** is an identifiable point on an object that corresponds to matching points on similar objects.
- This may be chosen based on the application (e.g., by anatomy) or mathematically (e.g., by curvature).

# Landmark Correspondence

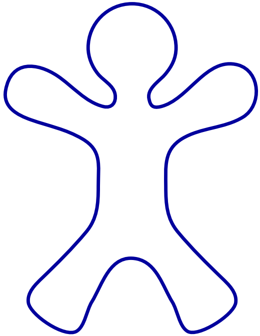


From C. Small, *The Statistical Theory of Shape*

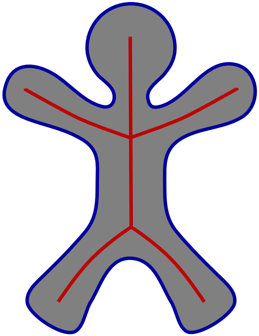
# More Geometry Representations



Dense Boundary
Points

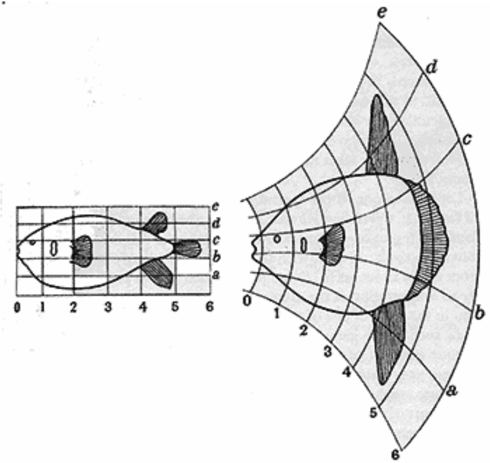


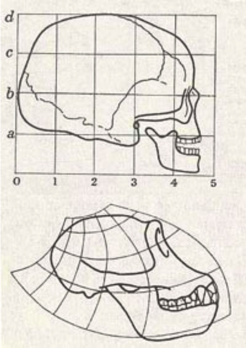
Continuous Boundary
(Fourier, splines)



Medial Axis
(solid interior)

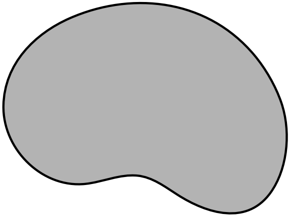
# Transformation Models



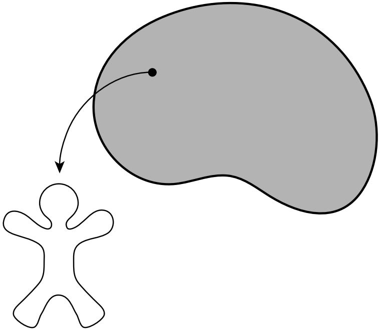

From D’Arcy Thompson, *On Growth and Form*, 1917.

# Shape Spaces



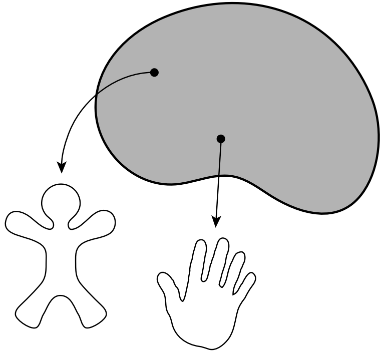
A shape is a point in a high-dimensional, nonlinear manifold, called a **shape space**.

# Shape Spaces



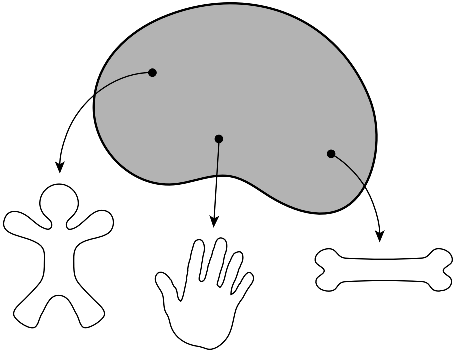
A shape is a point in a high-dimensional, nonlinear manifold, called a **shape space**.

# Shape Spaces



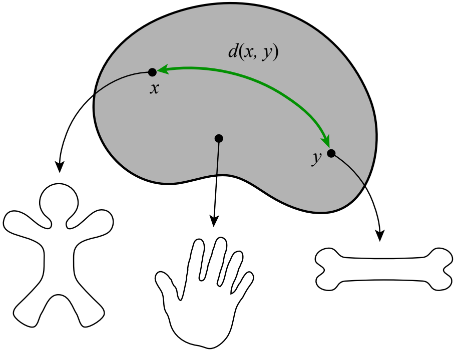
A shape is a point in a high-dimensional, nonlinear manifold, called a **shape space**.

# Shape Spaces



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

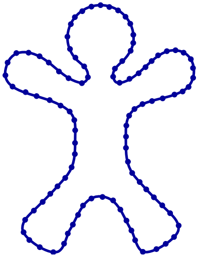
# Shape Spaces



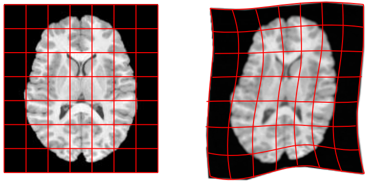

A metric space structure provides a comparison between two shapes.

# Examples: Shape Spaces

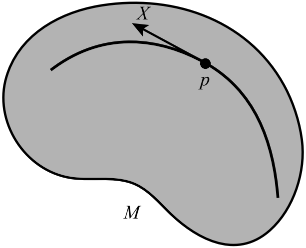
**Kendall's Shape Space**



**Space of Diffeomorphisms**

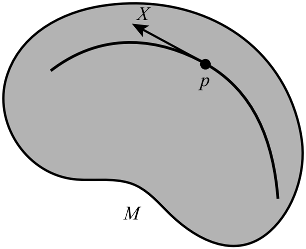


# Tangent Spaces

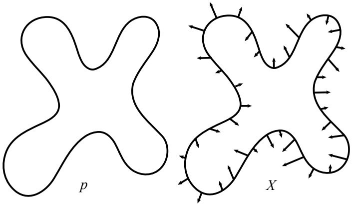



A **tangent vector** is the velocity of a curve on $M$.

# Tangent Spaces

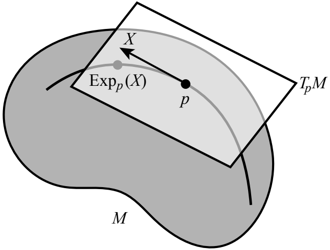



Infinitesimal change in shape:




A **tangent vector** is the velocity of a curve on $M$.

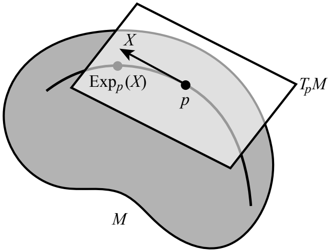
# The Exponential Map




Notation: $\mathrm{Exp}_p(X)$

- $p$: starting point on $M$
- $X$: initial velocity at $p$
- Output: endpoint of geodesic segment, starting at $p$, with velocity $X$, with same length as $\|X\|$

# The Log Map




Notation: $\mathrm{Log}_p(q)$

- Inverse of $\mathrm{Exp}$
- $p, q$: two points in $M$
- Output: tangent vector at $p$, such that $\mathrm{Exp}_p(\mathrm{Log}_p(q)) = q$
- Gives distance between points: $d(p,q) = \| \mathrm{Log}_p(q) \|$.

# Shape Equivalences

Two geometry representations, $x_1, x_2$, are **equivalent** if they are just a translation, rotation, scaling of each other:

$$x_2 = \lambda R \cdot x_1 + v,$$

where $\lambda$ is a scaling, $R$ is a rotation, and $v$ is a translation.

In notation: $x_1 \sim x_2$

# Equivalence Classes

The relationship $x_1 \sim x_2$ is an **equivalence relationship**:

- Reflexive: $x_1 \sim x_1$
- Symmetric: $x_1 \sim x_2$ implies $x_2 \sim x_1$
- Transitive: $x_1 \sim x_2$ and $x_2 \sim x_3$ imply $x_1 \sim x_3$

# Equivalence Classes

The relationship $x_1 \sim x_2$ is an **equivalence relationship**:

- Reflexive: $x_1 \sim x_1$
- Symmetric: $x_1 \sim x_2$ implies $x_2 \sim x_1$
- Transitive: $x_1 \sim x_2$ and $x_2 \sim x_3$ imply $x_1 \sim x_3$

We call the set of all equivalent geometries to $x$ the **equivalence class** of $x$:

$$[x] = \{y \,:\, y \sim x\}$$

# Equivalence Classes

The relationship $x_1 \sim x_2$ is an **equivalence relationship**:

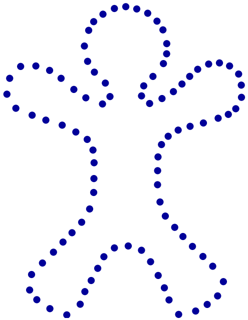
- Reflexive: $x_1 \sim x_1$
- Symmetric: $x_1 \sim x_2$ implies $x_2 \sim x_1$
- Transitive: $x_1 \sim x_2$ and $x_2 \sim x_3$ imply $x_1 \sim x_3$

We call the set of all equivalent geometries to $x$ the **equivalence class** of $x$:

$$[x] = \{y \,:\, y \sim x\}$$

The set of all equivalence classes is our **shape space**.

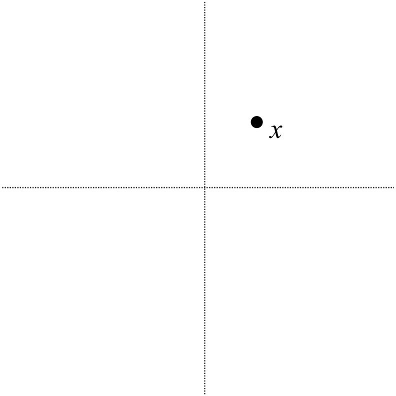
# Kendall's Shape Space



- Define object with $k$ points.
- Represent as a vector in $\mathbb{R}^{2k}$.
- Remove translation, rotation, and scale.
- End up with complex projective space, $\mathbb{CP}^{k-2}$.

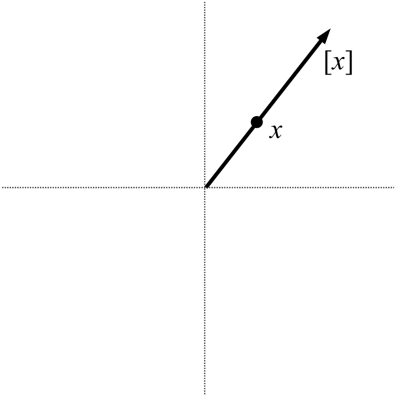
# Quotient Spaces

What do we get when we "remove" scaling from $\mathbb{R}^2$?



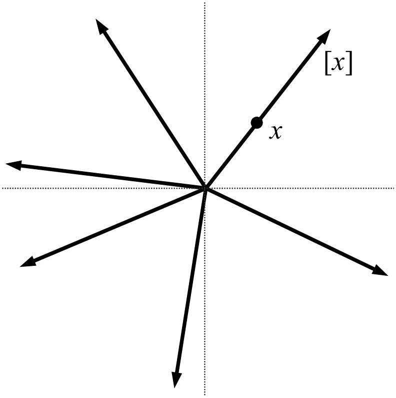
# Quotient Spaces

What do we get when we "remove" scaling from $\mathbb{R}^2$?



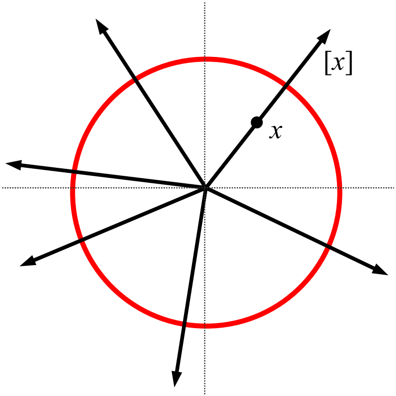
# Quotient Spaces

What do we get when we “remove” scaling from $\mathbb{R}^2$?



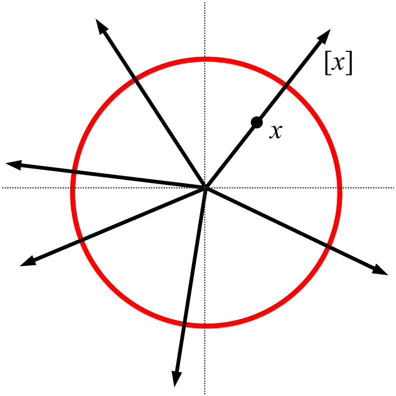
# Quotient Spaces

What do we get when we “remove” scaling from $\mathbb{R}^2$?



# Quotient Spaces

What do we get when we “remove” scaling from $\mathbb{R}^2$?




Notation: $[x] \in \mathbb{R}^2/\mathbb{R}^+$

# Constructing Kendall's Shape Space

- Consider planar landmarks to be points in the complex plane.

# Constructing Kendall's Shape Space

- Consider planar landmarks to be points in the complex plane.
- An object is then a point $(z_1, z_2, \ldots, z_k) \in \mathbb{C}^k$.

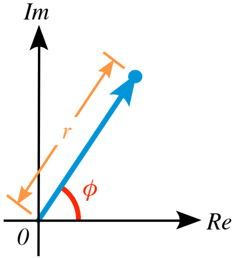
# Constructing Kendall's Shape Space

- Consider planar landmarks to be points in the complex plane.
- An object is then a point $(z_1, z_2, \ldots, z_k) \in \mathbb{C}^k$.
- Removing **translation** leaves us with $\mathbb{C}^{k-1}$.

# Constructing Kendall's Shape Space

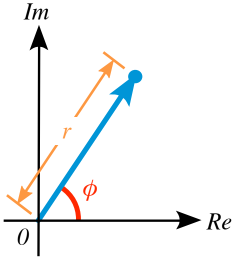
- Consider planar landmarks to be points in the complex plane.
- An object is then a point $(z_1, z_2, \ldots, z_k) \in \mathbb{C}^k$.
- Removing **translation** leaves us with $\mathbb{C}^{k-1}$.
- How to remove **scaling** and **rotation**?

# Scaling and Rotation in the Complex Plane




Recall a complex number can be written as $z = re^{i\phi}$, with modulus $r$ and argument $\phi$.

# Scaling and Rotation in the Complex Plane




Recall a complex number can be written as $z = re^{i\phi}$, with modulus $r$ and argument $\phi$.

Complex Multiplication:

$$se^{i\theta} * re^{i\phi} = (sr)e^{i(\theta+\phi)}$$

Multiplication by a complex number $se^{i\theta}$ is equivalent to scaling by $s$ and rotation by $\theta$.

# Removing Scale and Rotation

Multiplying a centered point set, $\mathbf{z} = (z_1, z_2, \ldots, z_{k-1})$, by a constant $w \in \mathbb{C}$, just rotates and scales it.

# Removing Scale and Rotation

Multiplying a centered point set, $\mathbf{z} = (z_1, z_2, \ldots, z_{k-1})$, by a constant $w \in \mathbb{C}$, just rotates and scales it.

Thus the shape of $\mathbf{z}$ is an equivalence class:

$$[\mathbf{z}] = \{(wz_1, wz_2, \ldots, wz_{k-1}) : \forall w \in \mathbb{C}\}$$

# Removing Scale and Rotation

Multiplying a centered point set, $\mathbf{z} = (z_1, z_2, \ldots, z_{k-1})$, by a constant $w \in \mathbb{C}$, just rotates and scales it.

Thus the shape of $\mathbf{z}$ is an equivalence class:

$$[\mathbf{z}] = \{(wz_1, wz_2, \ldots, wz_{k-1}) : \forall w \in \mathbb{C}\}$$

This gives complex projective space $\mathbb{CP}^{k-2}$ – much like the sphere comes from equivalence classes of scalar multiplication in $\mathbb{R}^n$.

# Alternative: Shape Matrices

Represent an object as a real $d \times k$ matrix.

**Preshape process:**

- Remove translation: subtract the row means from each row (i.e., translate shape centroid to 0).
- Remove scale: divide by the Frobenius norm.

# Orthogonal Procrustes Analysis

**Problem:**

Find the rotation $R^*$ that minimizes distance between two $d \times k$ matrices $A$, $B$:

$$R^* = \arg\min_{R \in \mathrm{SO}(d)} \|RA - B\|^2$$

# Orthogonal Procrustes Analysis

**Problem:**

Find the rotation $R^*$ that minimizes distance between two $d \times k$ matrices $A$, $B$:

$$R^* = \arg\min_{R \in \mathrm{SO}(d)} \|RA - B\|^2$$

**Solution:**

Let $U \Sigma V^T$ be the SVD of $BA^T$, then

$$R^* = UV^T$$

# Geodesics in 2D Kendall Shape Space

Let $A$ and $B$ be $2 \times k$ shape matrices

1. Remove centroids from $A$ and $B$

# Geodesics in 2D Kendall Shape Space

Let $A$ and $B$ be $2 \times k$ shape matrices

1. Remove centroids from $A$ and $B$
2. Project onto sphere: $A \leftarrow A/\|A\|$, $B \leftarrow B/\|B\|$

# Geodesics in 2D Kendall Shape Space

Let $A$ and $B$ be $2 \times k$ shape matrices

1. Remove centroids from $A$ and $B$
2. Project onto sphere: $A \leftarrow A/\|A\|$, $B \leftarrow B/\|B\|$
3. Align rotation of $B$ to $A$ with OPA

# Geodesics in 2D Kendall Shape Space

Let $A$ and $B$ be $2 \times k$ shape matrices

1. Remove centroids from $A$ and $B$
2. Project onto sphere: $A \leftarrow A/\|A\|$, $B \leftarrow B/\|B\|$
3. Align rotation of $B$ to $A$ with OPA
4. Now a geodesic is simply that of the sphere, $S^{2k-1}$

# Intrinsic Means (Fréchet)

The *intrinsic mean* of a collection of points $x_1, \ldots, x_N$ in a metric space $M$ is

$$\mu = \arg\min_{x \in M} \sum_{i=1}^{N} d(x, x_i)^2,$$

where $d(\cdot, \cdot)$ denotes distance in $M$.

# Gradient of the Geodesic Distance

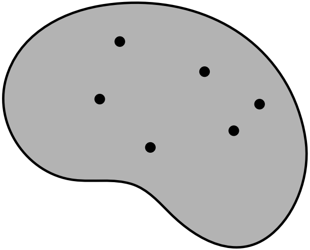
The gradient of the Riemannian distance function is

$$\mathrm{grad}_x d(x, y)^2 = -2 \operatorname{Log}_x(y).$$

So, gradient of the sum-of-squared distance function is

$$\mathrm{grad}_x \sum_{i=1}^{N} d(x, x_i)^2 = -2 \sum_{i=1}^{N} \operatorname{Log}_x(x_i).$$

# Computing Means



**Gradient Descent Algorithm:**

Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

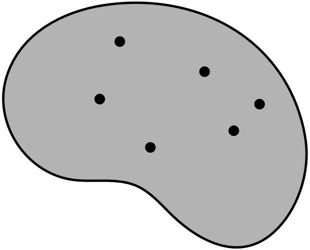
$\mu_0 = \mathbf{x}_1$

Repeat:

$$\delta\mu = \frac{1}{N} \sum_{i=1}^{N} \mathrm{Log}_{\mu_k}(\mathbf{x}_i)$$

$$\mu_{k+1} = \mathrm{Exp}_{\mu_k}(\delta\mu)$$

# Computing Means



**Gradient Descent Algorithm:**

Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

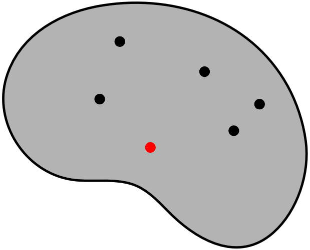
$\mu_0 = \mathbf{x}_1$

Repeat:

$$\delta\mu = \frac{1}{N} \sum_{i=1}^{N} \mathrm{Log}_{\mu_k}(\mathbf{x}_i)$$

$$\mu_{k+1} = \mathrm{Exp}_{\mu_k}(\delta\mu)$$

# Computing Means



**Gradient Descent Algorithm:**

Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

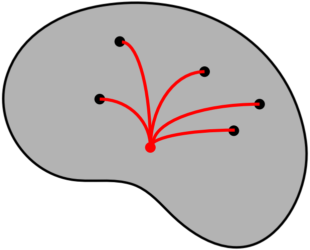
$\mu_0 = \mathbf{x}_1$

Repeat:

$$\delta\mu = \frac{1}{N}\sum_{i=1}^{N} \mathrm{Log}_{\mu_k}(\mathbf{x}_i)$$

$$\mu_{k+1} = \mathrm{Exp}_{\mu_k}(\delta\mu)$$

# Computing Means



**Gradient Descent Algorithm:**

Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

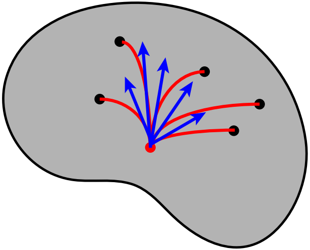
$\mu_0 = \mathbf{x}_1$

Repeat:

$$\delta\mu = \frac{1}{N} \sum_{i=1}^{N} \mathrm{Log}_{\mu_k}(\mathbf{x}_i)$$

$$\mu_{k+1} = \mathrm{Exp}_{\mu_k}(\delta\mu)$$

# Computing Means



**Gradient Descent Algorithm:**

Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

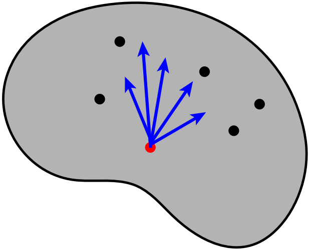
$\mu_0 = \mathbf{x}_1$

Repeat:

$$\delta\mu = \frac{1}{N} \sum_{i=1}^{N} \mathrm{Log}_{\mu_k}(\mathbf{x}_i)$$

$$\mu_{k+1} = \mathrm{Exp}_{\mu_k}(\delta\mu)$$

# Computing Means



**Gradient Descent Algorithm:**

Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

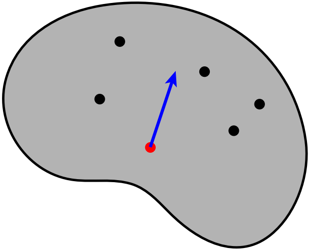
$\mu_0 = \mathbf{x}_1$

Repeat:

$$\delta\mu = \frac{1}{N} \sum_{i=1}^{N} \mathrm{Log}_{\mu_k}(\mathbf{x}_i)$$

$$\mu_{k+1} = \mathrm{Exp}_{\mu_k}(\delta\mu)$$

# Computing Means



**Gradient Descent Algorithm:**

Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

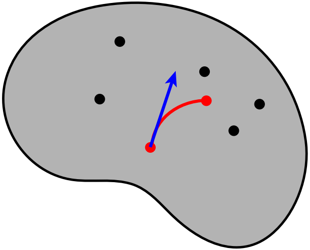
$\mu_0 = \mathbf{x}_1$

Repeat:

$$\delta\mu = \frac{1}{N} \sum_{i=1}^{N} \mathrm{Log}_{\mu_k}(\mathbf{x}_i)$$

$$\mu_{k+1} = \mathrm{Exp}_{\mu_k}(\delta\mu)$$

# Computing Means



**Gradient Descent Algorithm:**

Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

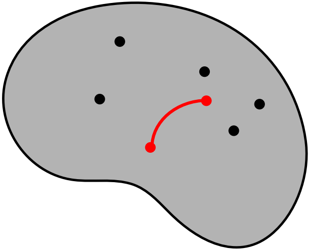
$\mu_0 = \mathbf{x}_1$

Repeat:

$$\delta\mu = \frac{1}{N} \sum_{i=1}^{N} \mathrm{Log}_{\mu_k}(\mathbf{x}_i)$$

$$\mu_{k+1} = \mathrm{Exp}_{\mu_k}(\delta\mu)$$

# Computing Means



**Gradient Descent Algorithm:**

Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

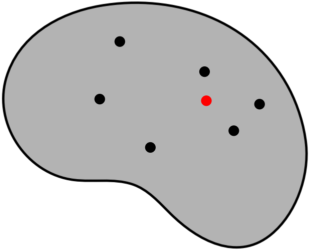
$\mu_0 = \mathbf{x}_1$

Repeat:

$$\delta\mu = \frac{1}{N} \sum_{i=1}^{N} \mathrm{Log}_{\mu_k}(\mathbf{x}_i)$$

$$\mu_{k+1} = \mathrm{Exp}_{\mu_k}(\delta\mu)$$

# Computing Means



**Gradient Descent Algorithm:**

Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

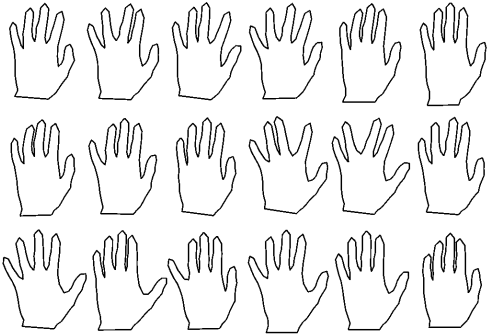
$\mu_0 = \mathbf{x}_1$

Repeat:

$$\delta\mu = \frac{1}{N} \sum_{i=1}^{N} \mathrm{Log}_{\mu_k}(\mathbf{x}_i)$$

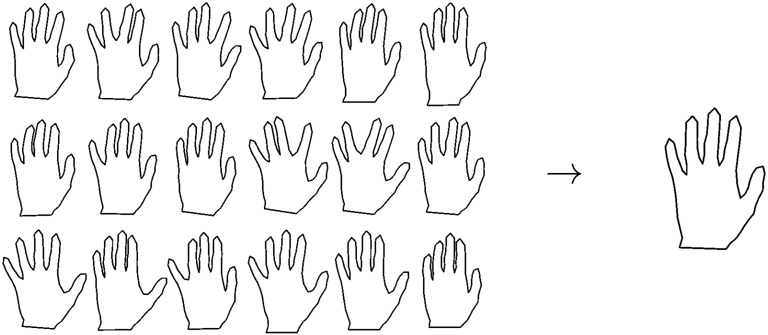
$$\mu_{k+1} = \mathrm{Exp}_{\mu_k}(\delta\mu)$$

# Example of Mean on Kendall Shape Space



Hand data from Tim Cootes

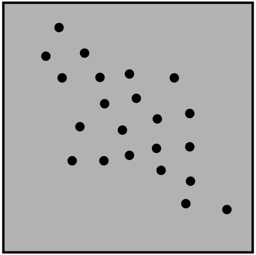
# Example of Mean on Kendall Shape Space



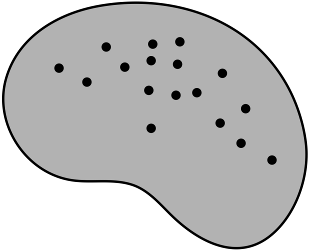
Hand data from Tim Cootes

# Principal Geodesic Analysis

Linear Statistics (PCA)

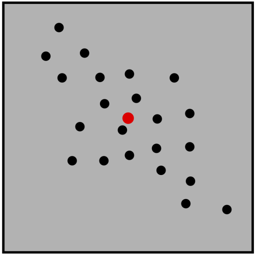


Curved Statistics (PGA)

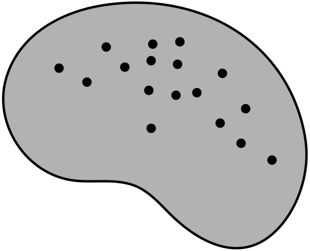


# Principal Geodesic Analysis

Linear Statistics (PCA)

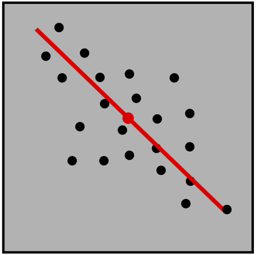


Curved Statistics (PGA)

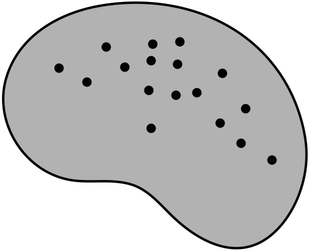


# Principal Geodesic Analysis

Linear Statistics (PCA)

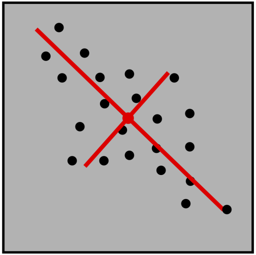


Curved Statistics (PGA)

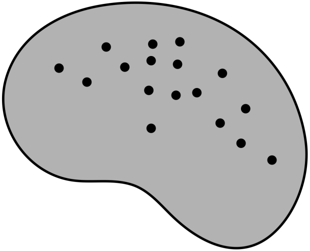


# Principal Geodesic Analysis

Linear Statistics (PCA)

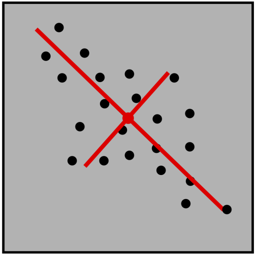


Curved Statistics (PGA)

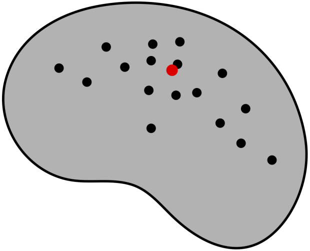


# Principal Geodesic Analysis

Linear Statistics (PCA)

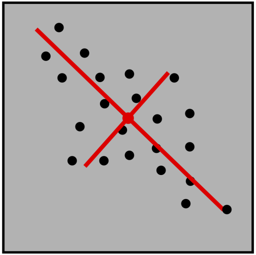


Curved Statistics (PGA)

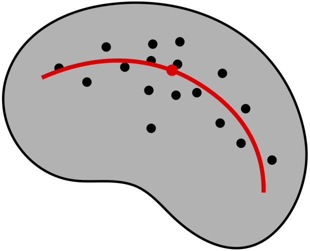


# Principal Geodesic Analysis

Linear Statistics (PCA)

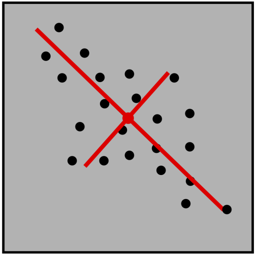


Curved Statistics (PGA)

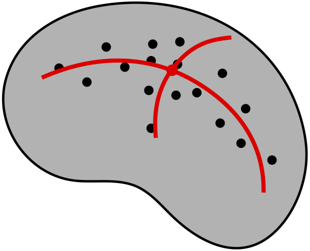


# Principal Geodesic Analysis

Linear Statistics (PCA)



Curved Statistics (PGA)



# PGA of Kidney

Mode 1 Mode 2 Mode 3

# PGA Definition

First principal geodesic direction:

$$v_1 = \arg\max_{\|v\|=1} \sum_{i=1}^{N} \| \operatorname{Log}_{\bar{y}}(\pi_H(y_i)) \|^2,$$

where $\quad H = \operatorname{Exp}_{\bar{y}}(\operatorname{span}(\{v\}) \cap U).$

# PGA Definition

First principal geodesic direction:

$$v_1 = \arg\max_{\|v\|=1} \sum_{i=1}^{N} \| \operatorname{Log}_{\bar{y}}(\pi_H(y_i)) \|^2,$$

where $\quad H = \operatorname{Exp}_{\bar{y}}(\operatorname{span}(\{v\}) \cap U).$

Remaining principal directions are defined recursively as

$$v_k = \arg\max_{\|v\|=1} \sum_{i=1}^{N} \| \operatorname{Log}_{\bar{y}}(\pi_H(y_i)) \|^2,$$

where $\quad H = \operatorname{Exp}_{\bar{y}}(\operatorname{span}(\{v_1, \ldots, v_{k-1}, v\}) \cap U).$

# Tangent Approximation to PGA

**Input:** Data $y_1, \ldots, y_N \in M$

**Output:** Principal directions, $v_k \in T_\mu M$, variances, $\lambda_k \in \mathbb{R}$

$\bar{y} =$ Fréchet mean of $\{y_i\}$

$u_i = \mathrm{Log}_\mu(y_i)$

$\mathbf{S} = \frac{1}{N-1} \sum_{i=1}^{N} u_i u_i^T$

$\{v_k, \lambda_k\}$ = eigenvectors/eigenvalues of $\mathbf{S}$.

# Where to Learn More

## Books


- Dryden and Mardia, *Statistical Shape Analysis*, Wiley, 1998.
- Small, *The Statistical Theory of Shape*, Springer-Verlag, 1996.
- Kendall, Barden and Carne, *Shape and Shape Theory*, Wiley, 1999.
- Krim and Yezzi, *Statistics and Analysis of Shapes*, Birkhauser, 2006.