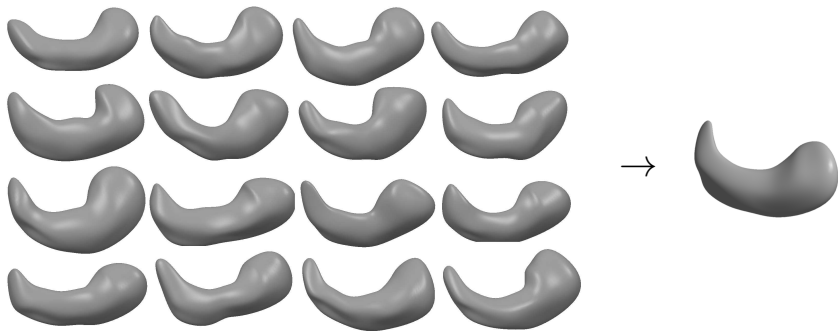# Introduction to Shape Manifolds
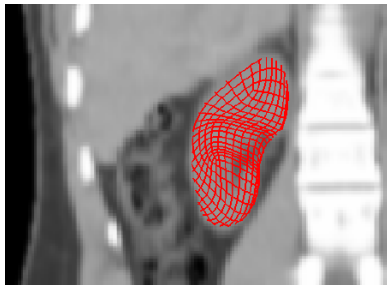
Geometry of Data

September 26, 2019

Shape Statistics: Averages
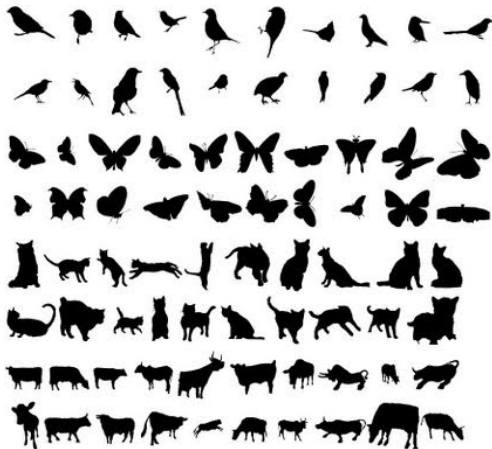
Shape Statistics: Variability

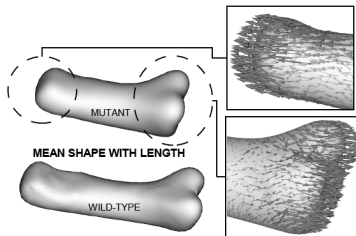Shape priors in segmentation

Shape Statistics: Classification

http://sites.google.com/site/xiangbai/animaldataset
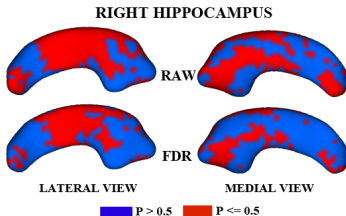
Shape Statistics: Hypothesis Testing

Testing group differences

Cates, et al. IPMI 2007 and ISBI 2008

Shape Application: Bird Identification

American Crow

Common Raven

Shape Application: Bird Identification
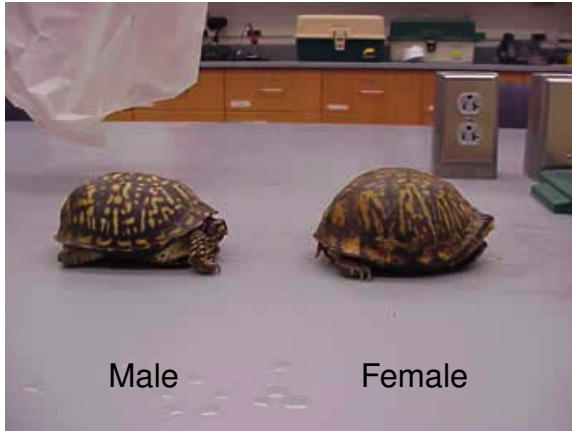
Glaucous Gull

Iceland Gull

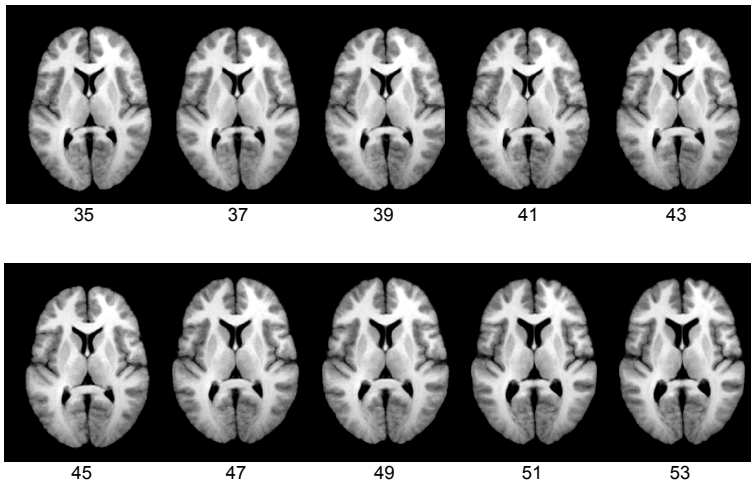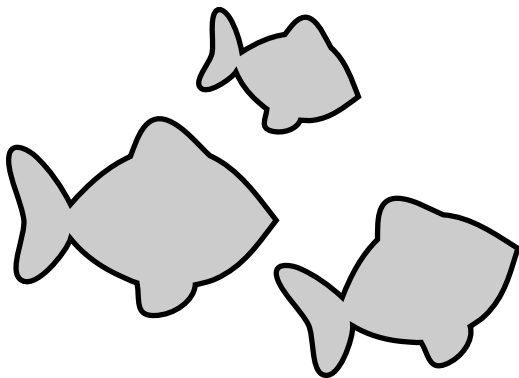http://notendur.hi.is/yannk/specialities.htm

Shape Application: Box Turtles

Male   Female

Shape Statistics: Regression

35 37 39 41 43
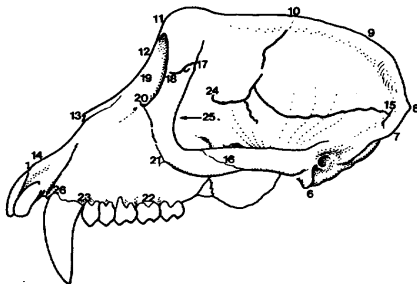
45 47 49 51 53

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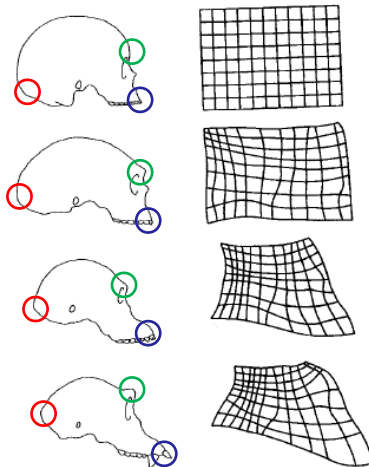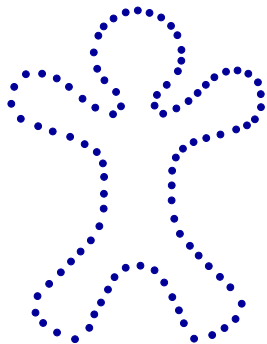
- ▶ A **landmark** is an identifiable point on an object that corresponds to matching points on similar objects.
- ▶ This may be chosen based on the application (e.g., by anatomy) or mathematically (e.g., by curvature).
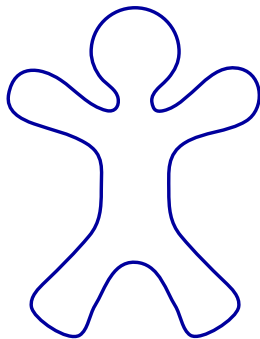
Landmark Correspondence

More Geometry Representations
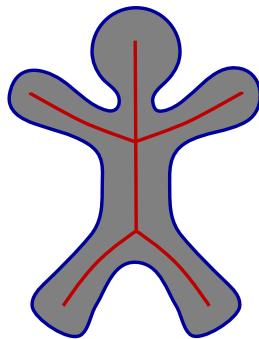

Dense Boundary
Points

Continuous Boundary
(Fourier, splines)

Medial Axis
(solid interior)

Transformation Models
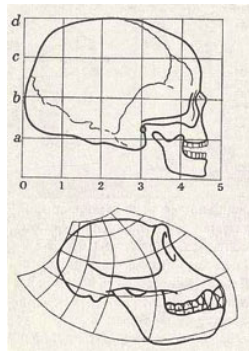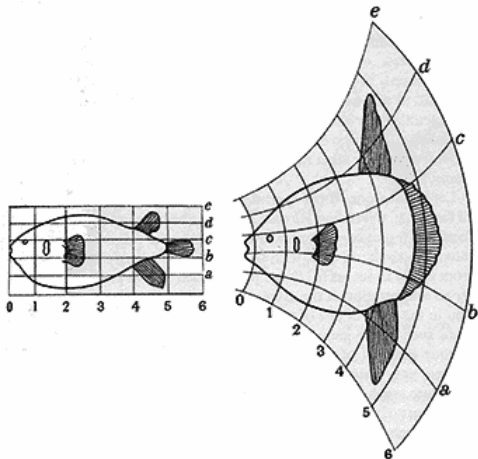
From D'Arcy Thompson, *On Growth and Form*, 1917.

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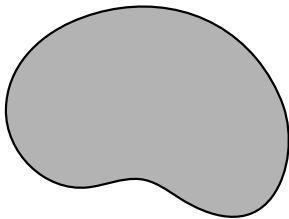
A shape is a point in a high-dimensional, nonlinear manifold, called a **shape space**.
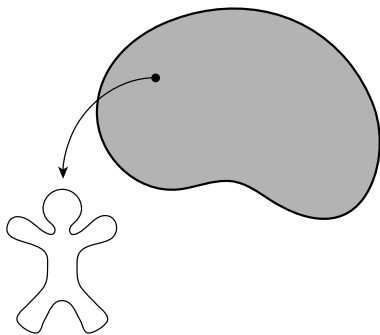
Shape Spaces

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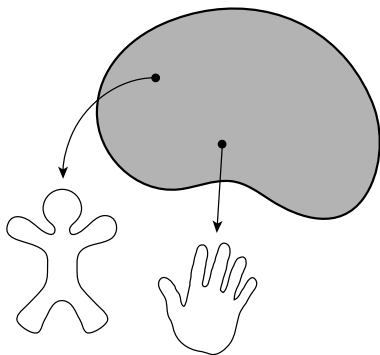
Shape Spaces

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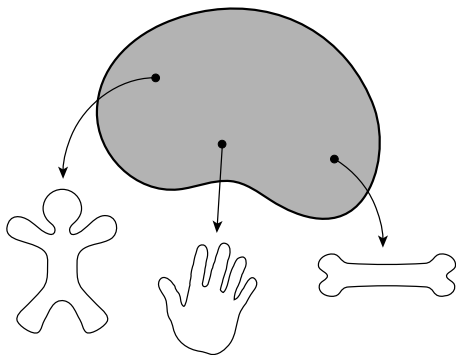
Shape Spaces

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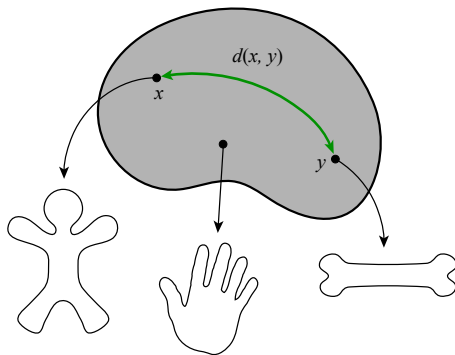
Shape Spaces

A metric space structure provides a comparison
between two shapes.

Examples: Shape Spaces

Kendall's Shape Space
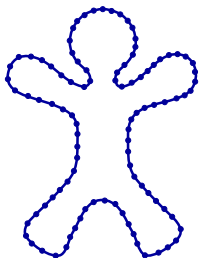
Space of Diffeomorphisms
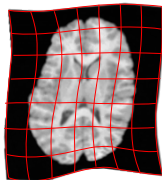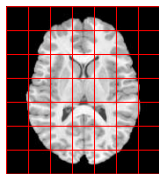
Tangent Spaces
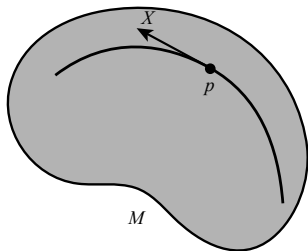
Infinitesimal change in shape:
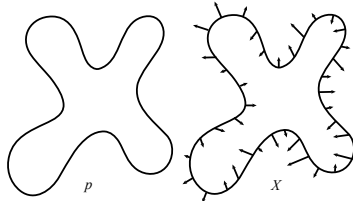
A **tangent vector** is the velocity of a curve on M.

The Exponential Map
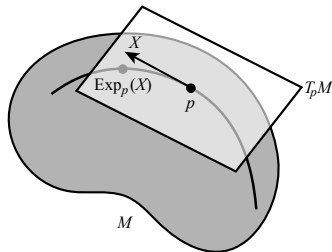
Notation: $\text{Exp}_p(X)$

▶ 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
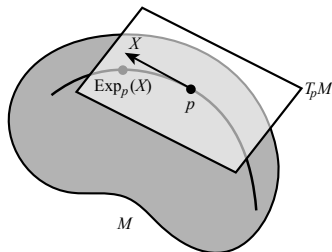
Notation: $\mathrm{Log}_p(q)$

▶ Inverse of 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 λ 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 $x_1 \sim x_3$

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

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

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

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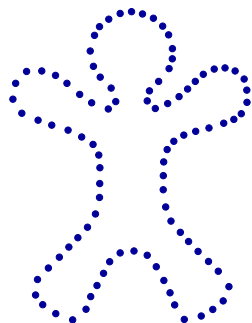
- ▶ Define object with k points.
- ▶ Represent as a vector in $\mathbb{R}^{2k}$.
- ▶ Remove translation, rotation, and scale.
- ▶ End up with complex projective space, $\mathbb{CP}^{k-2}$.

Quotient Spaces

What do we get when we "remove" scaling from $\mathbb{R}^2$?
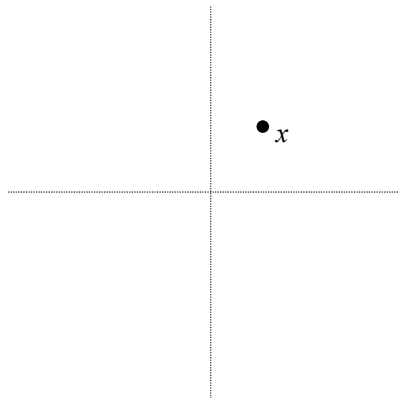
Notation: $[x] \in \mathbb{R}^2/\mathbb{R}^+$

Quotient Spaces

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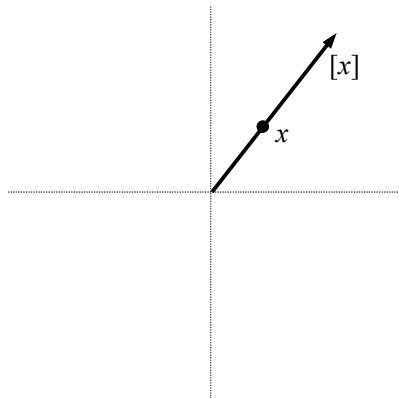
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Quotient Spaces

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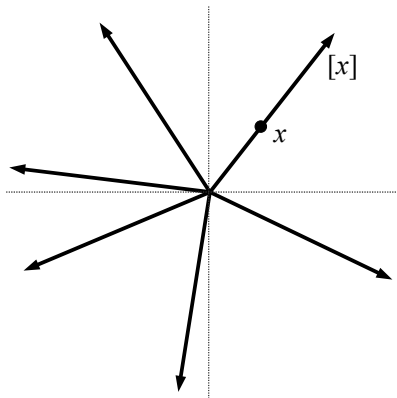
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Quotient Spaces

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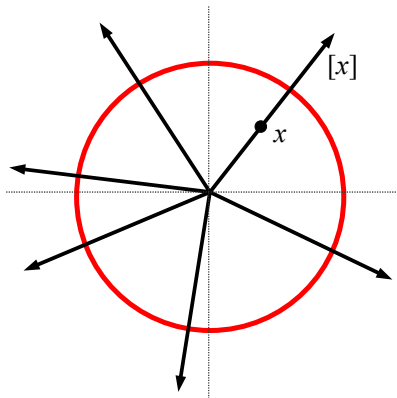
Notation: $[x] \in \mathbb{R}^2/\mathbb{R}^+$

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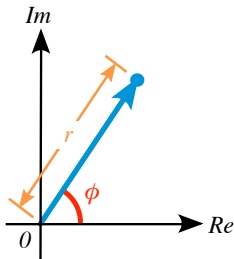
Recall a complex number can be written as $z = re^{i\phi}$, with modulus r and argument ϕ.

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 θ.

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:

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

Solution:

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

$$R^* = UV^T$$

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.
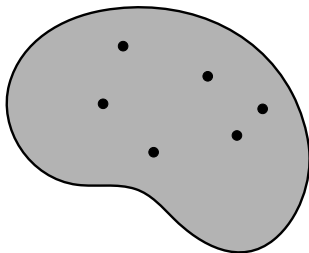
Gradient of the Geodesic Distance

The gradient of the Riemannian distance function is

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

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

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

Computing Means

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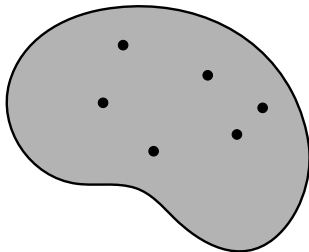
Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

$\mu_0 = \mathbf{x}_1$

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:
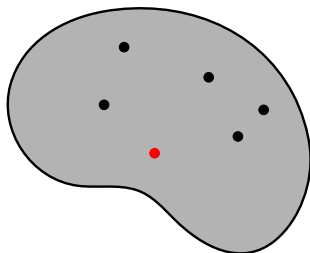
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Computing Means

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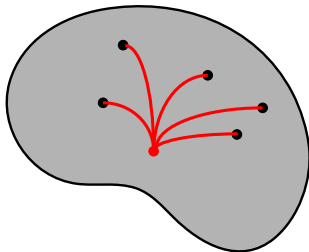
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Gradient Descent Algorithm:

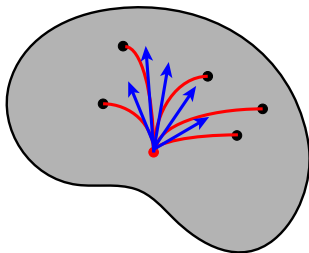Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

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Computing Means

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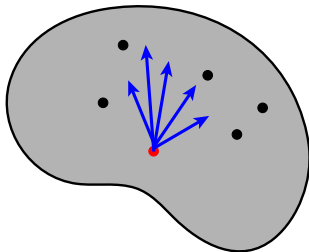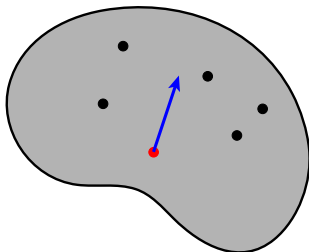Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

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Computing Means

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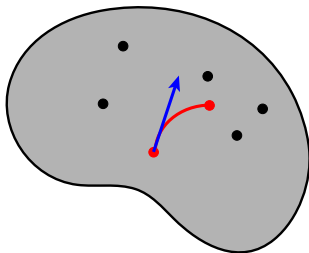
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Computing Means

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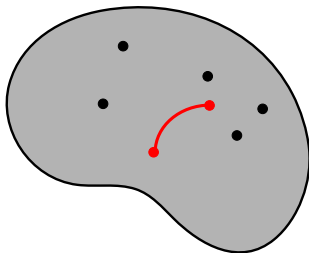
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Computing Means

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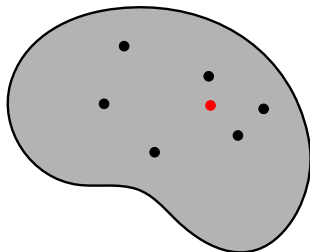
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Gradient Descent Algorithm:

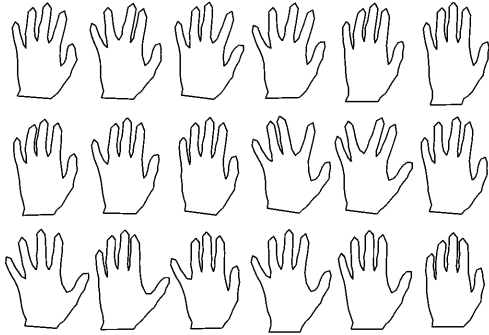Input: $\mathbf{x}_1, \ldots, \mathbf{x}_N \in M$

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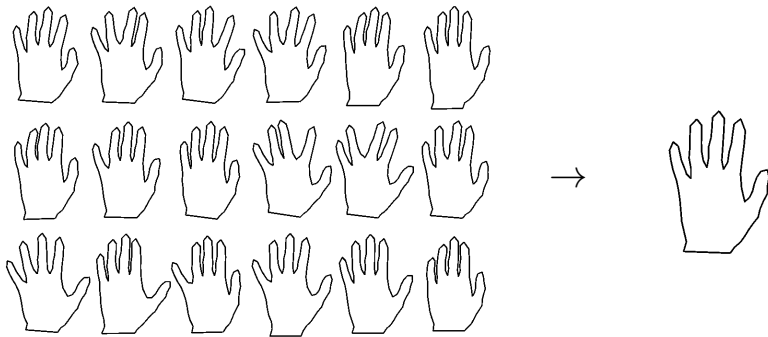$$\delta\mu = \frac{1}{N}\sum_{i=1}^{N}\mathrm{Log}_{\mu_k}(\mathbf{x}_i)$$

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Example of Mean on Kendall Shape Space
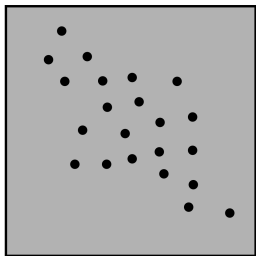

Hand data from Tim Cootes

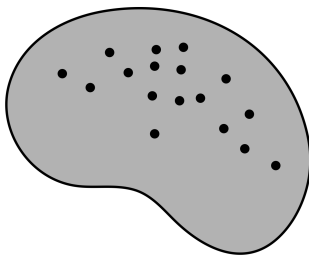# Example of Mean on Kendall Shape Space

Hand data from Tim Cootes

Principal Geodesic Analysis
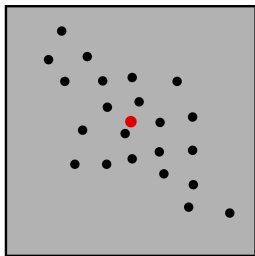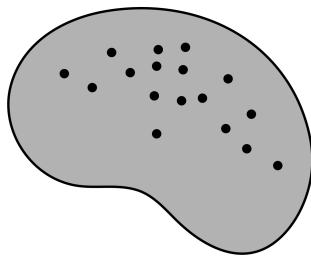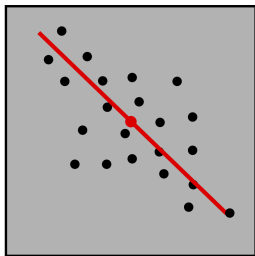

Linear Statistics (PCA)   Curved Statistics (PGA)

Principal Geodesic Analysis

Linear Statistics (PCA)   Curved Statistics (PGA)

Principal Geodesic Analysis

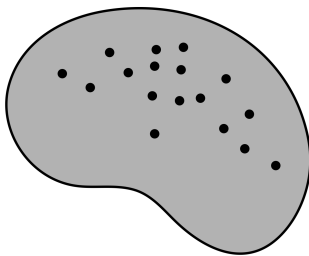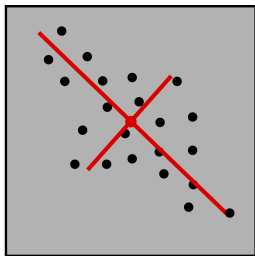Linear Statistics (PCA)   Curved Statistics (PGA)

Principal Geodesic Analysis

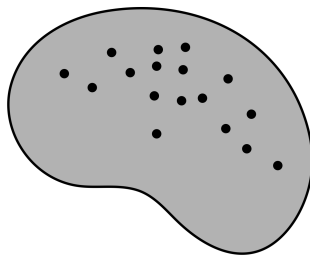Linear Statistics (PCA)   Curved Statistics (PGA)

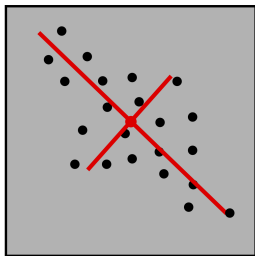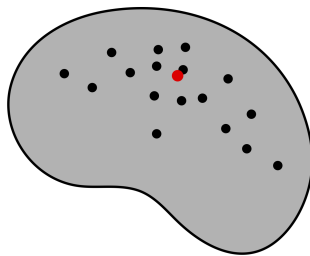# Principal Geodesic Analysis

Linear Statistics (PCA) Curved Statistics (PGA)

Principal Geodesic Analysis

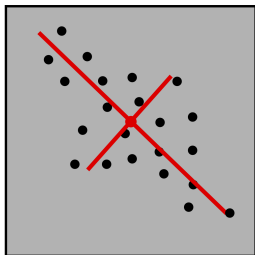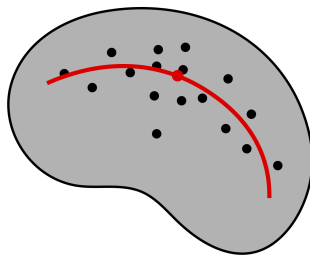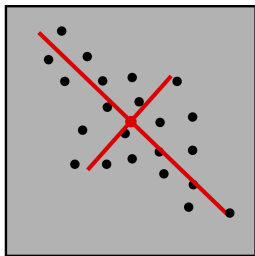Linear Statistics (PCA)   Curved Statistics (PGA)
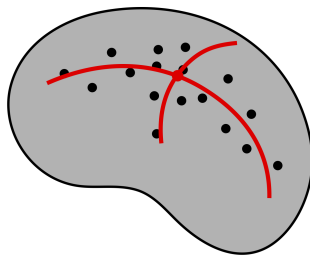
Principal Geodesic Analysis

Linear Statistics (PCA)　　　　Curved Statistics (PGA)

PGA of Kidney

Mode 1   Mode 2   Mode 3

PGA Definition

First principal geodesic direction:

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

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

Remaining principal directions are defined recursively as

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

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

Tangent Approximation to PGA

Input: Data $y_1, \ldots, y_N \in M$
Output: Principal directions, $v_k \in T_\mu M$, variances,
$\quad \quad \lambda_k \in \mathbb{R}$
$\bar{y} =$ Fréchet mean of $\{y_i\}$
$u_i = \text{Log}_\mu(y_i)$
$\mathbf{S} = \frac{1}{N-1} \sum_{i=1}^{N} u_i u_i^T$
$\{v_k, \lambda_k\}$ = 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.