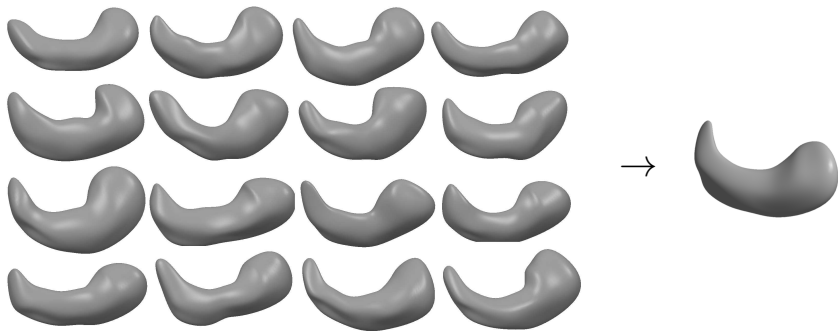


Introduction to Shape Manifolds

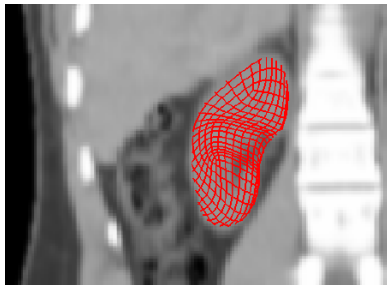
Geometry of Data

September 26, 2019

Shape Statistics: Averages

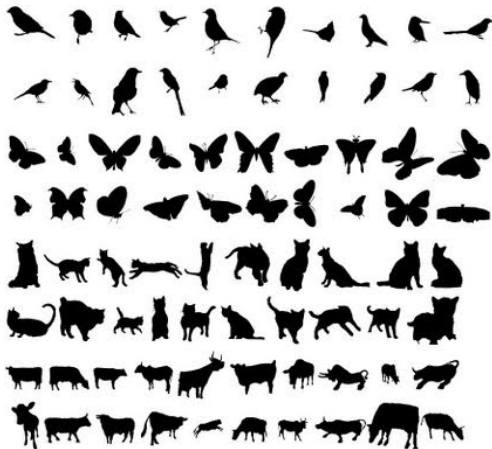


Shape Statistics: Variability



Shape priors in segmentation

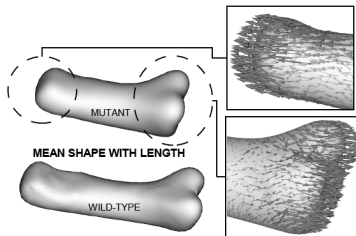
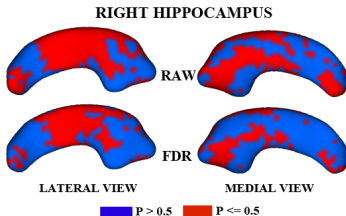
Shape Statistics: Classification



<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

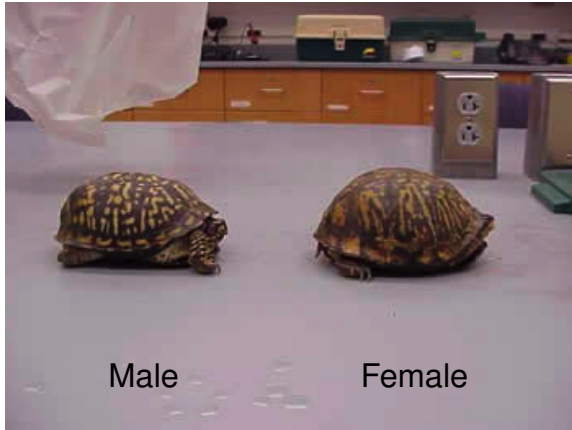


Iceland Gull



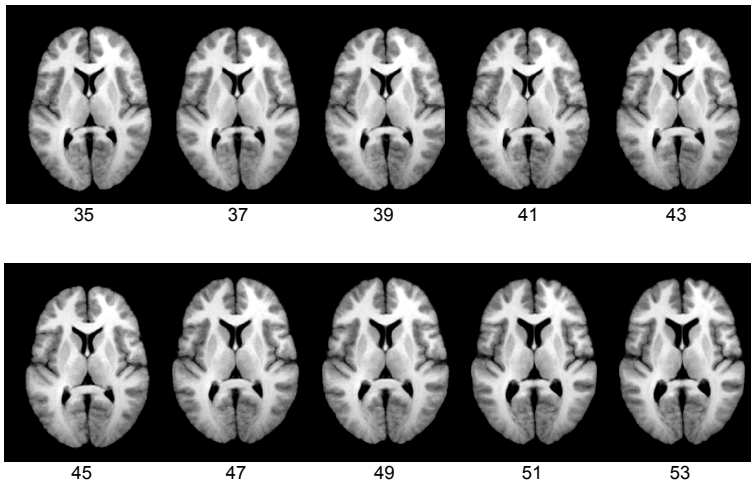
<http://notendur.hi.is/yannk/specialities.htm>

Shape Application: Box Turtles

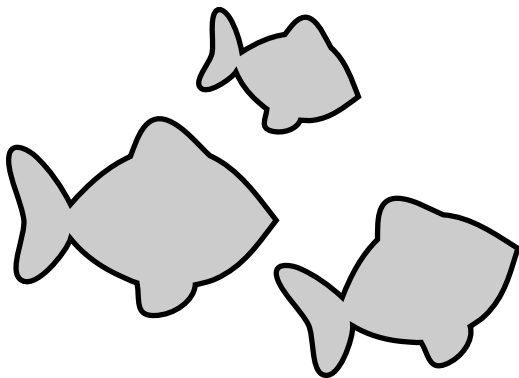


<http://www.bio.davidson.edu/people/midorcas/research/Contribute/boxturtle/boxinfo.htm>

Shape Statistics: Regression



What is Shape?

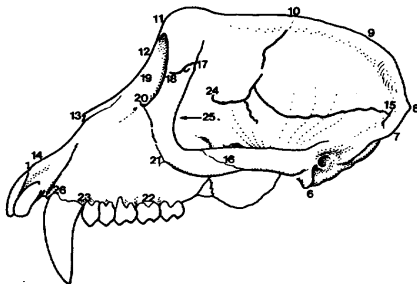


Shape is the geometry of an object modulo position, orientation, and size.

Geometry Representations

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

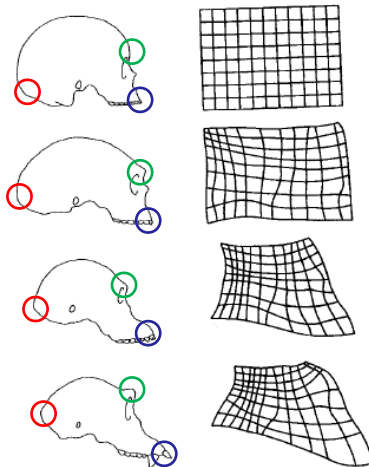
Landmarks



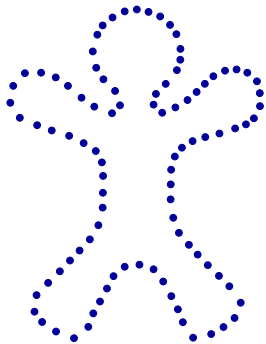
From Dryden & Mardia, 1998

- ▶ 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).

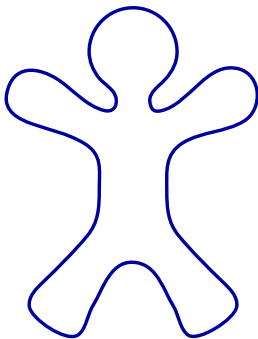
Landmark Correspondence



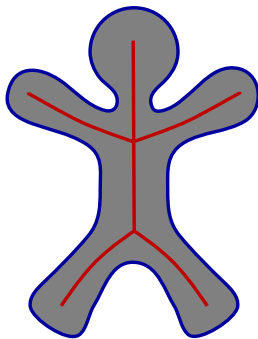
More Geometry Representations



Dense Boundary
Points

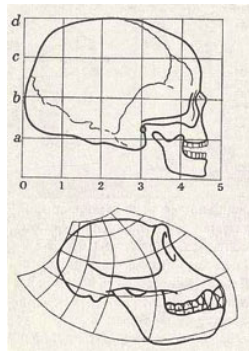
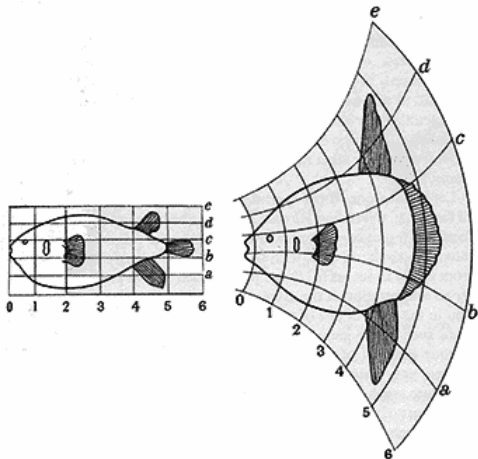


Continuous Boundary
(Fourier, splines)



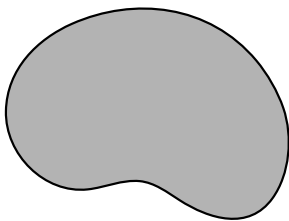
Medial Axis
(solid interior)

Transformation Models



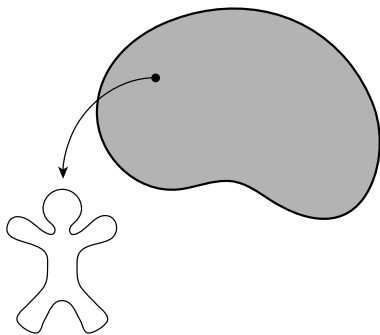
From D'Arcy Thompson, *On Growth and Form*, 1917.

Shape Spaces



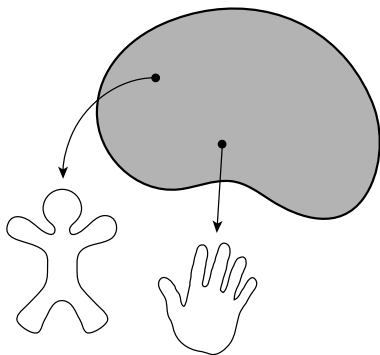
A shape is a point in a high-dimensional, nonlinear manifold, called a **shape space**.

Shape Spaces



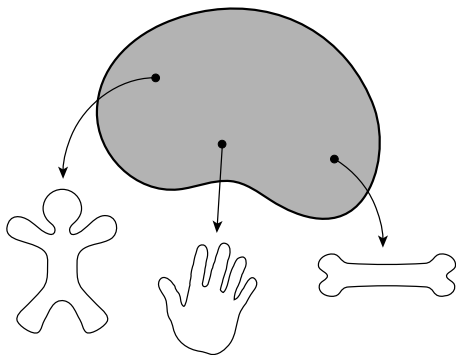
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Shape Spaces



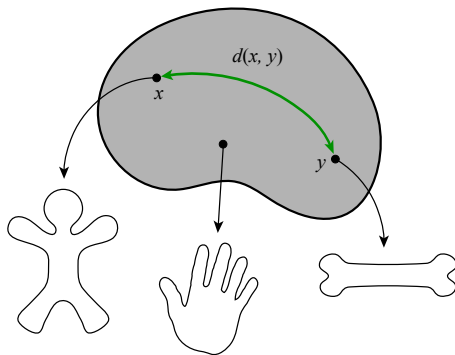
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Shape Spaces



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

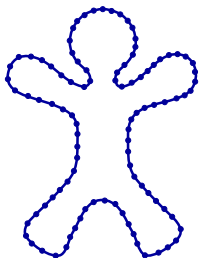
Shape Spaces



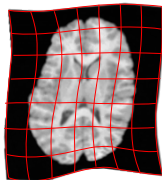
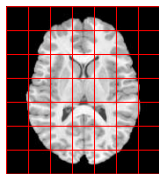
A metric space structure provides a comparison between two shapes.

Examples: Shape Spaces

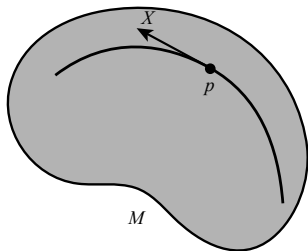
Kendall's Shape Space



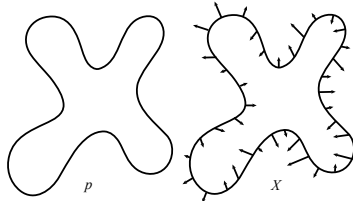
**Space of
Diffeomorphisms**



Tangent Spaces

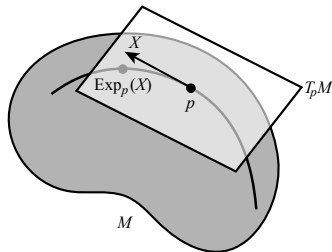


Infinitesimal change in shape:



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

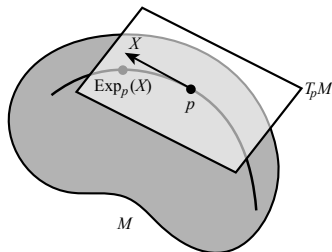
The Exponential Map



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: $\text{Log}_p(q)$

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

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**:

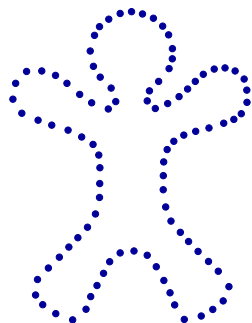
- ▶ Reflexive: $x_1 \sim x_1$
- ▶ Symmetric: $x_1 \sim x_2$ implies $x_2 \sim x_1$
- ▶ Transitive: $x_1 \sim x_2$ and $x_2 \sim x_3$ imply $x_1 \sim x_3$

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

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

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

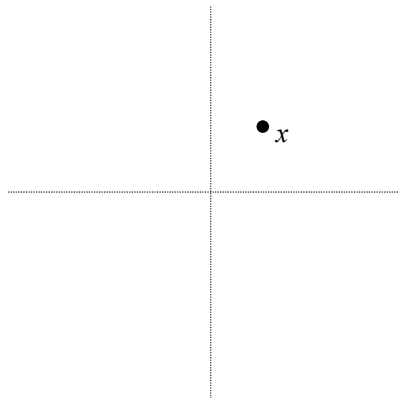
Kendall's Shape Space



- ▶ 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

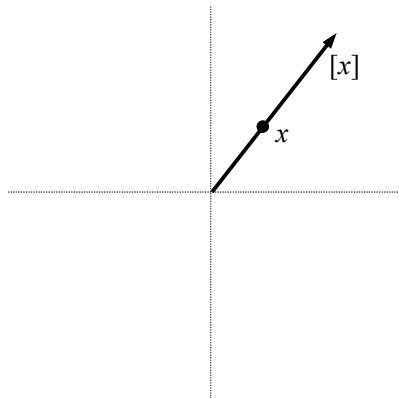
What do we get when we “remove” scaling from \mathbb{R}^2 ?



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

Quotient Spaces

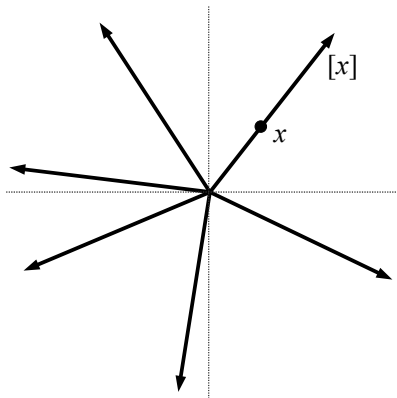
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Quotient Spaces

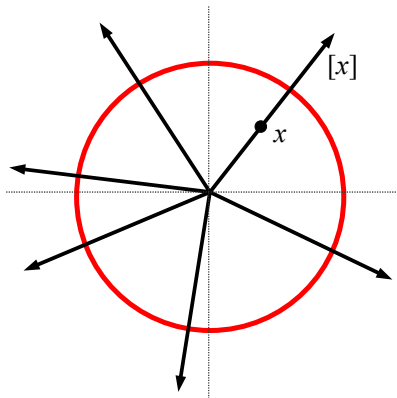
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Quotient Spaces

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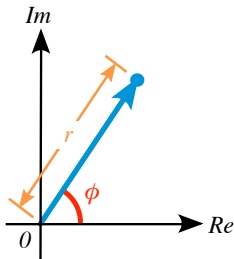


Notation: $[x] \in \mathbb{R}^2 / \mathbb{R}^+$

Constructing Kendall's Shape Space

- ▶ Consider planar landmarks to be points in the complex plane.
- ▶ An object is then a point $(z_1, z_2, \dots, z_k) \in \mathbb{C}^k$.
- ▶ 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, $\mathbf{z} = (z_1, z_2, \dots, z_{k-1})$, by a constant $w \in \mathbb{C}$, just rotates and scales it.

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

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

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 :

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

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
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, \dots, 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

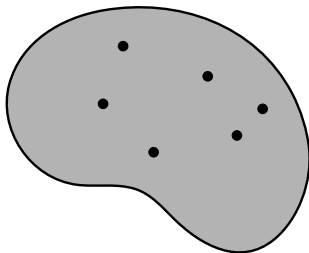
The gradient of the Riemannian distance function is

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

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

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

Computing Means



Gradient Descent Algorithm:

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

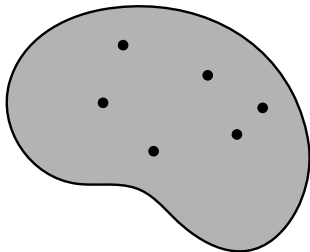
$$\mu_0 = \mathbf{x}_1$$

Repeat:

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

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

Computing Means



Gradient Descent Algorithm:

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

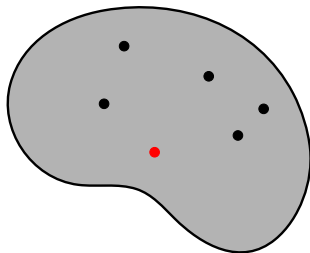
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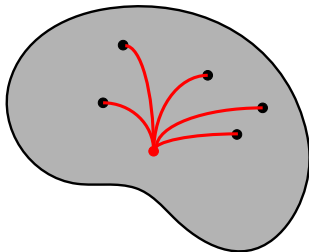
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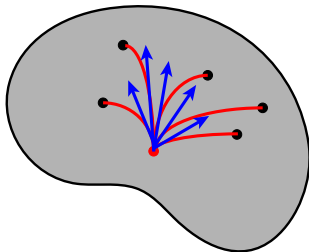
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Computing Means



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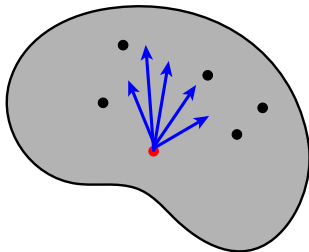
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Computing Means



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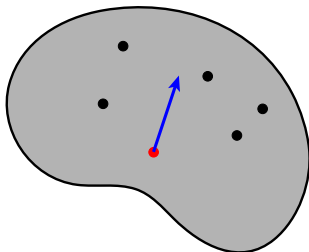
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Gradient Descent Algorithm:

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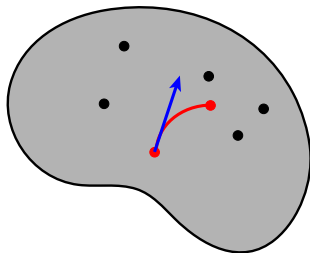
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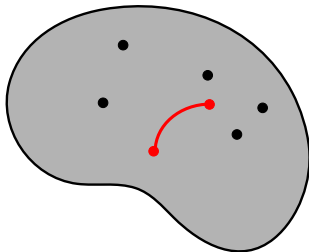
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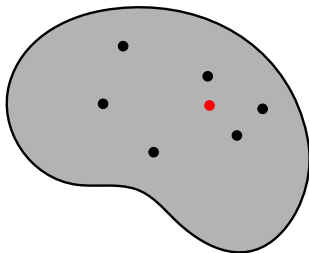
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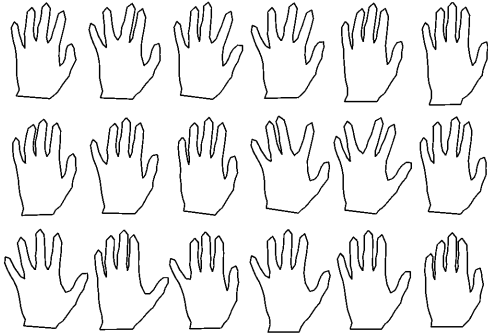
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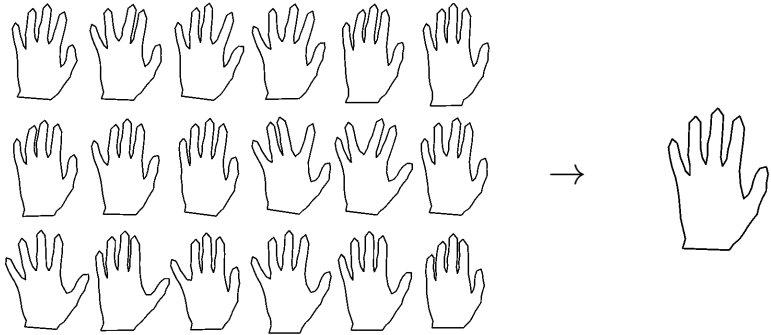
$$\mu_{k+1} = \text{Exp}_{\mu_k}(\delta\mu)$$

Example of Mean on Kendall Shape Space



Hand data from Tim Cootes

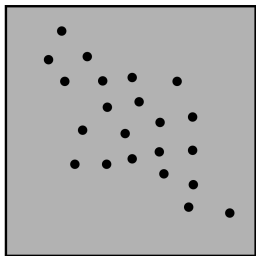
Example of Mean on Kendall Shape Space



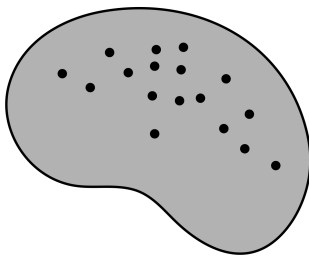
Hand data from Tim Cootes

Principal Geodesic Analysis

Linear Statistics (PCA)

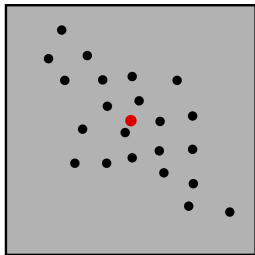


Curved Statistics (PGA)

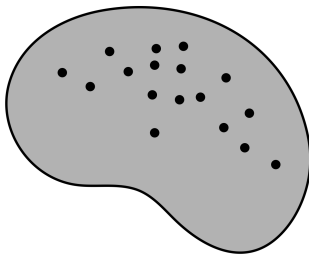


Principal Geodesic Analysis

Linear Statistics (PCA)

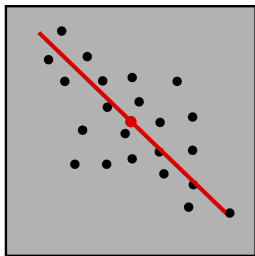


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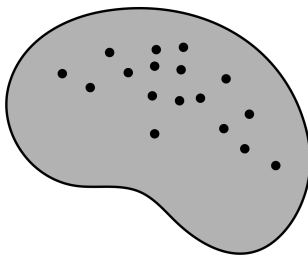


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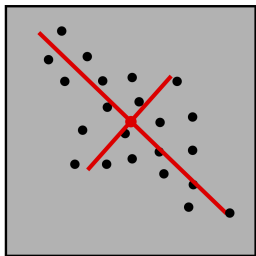


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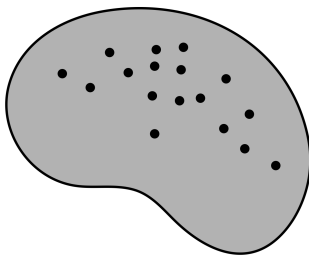


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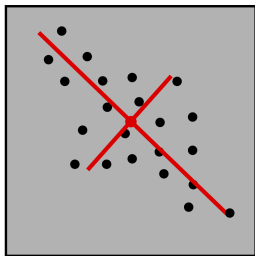


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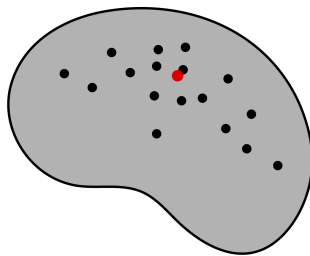


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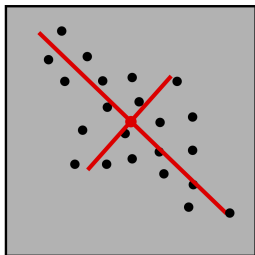


Curved Statistics (PGA)

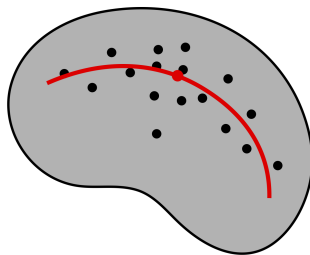


Principal Geodesic Analysis

Linear Statistics (PCA)

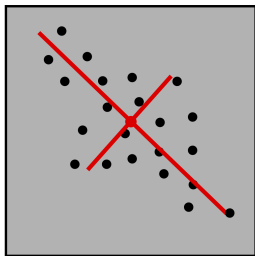


Curved Statistics (PGA)

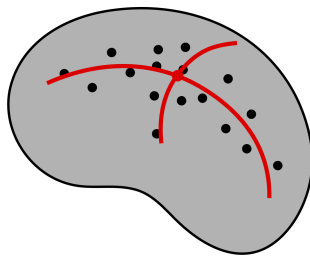


Principal Geodesic Analysis

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

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

Tangent Approximation to PGA

Input: Data $y_1, \dots, y_N \in M$

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

\bar{y} = Fréchet mean of $\{y_i\}$

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

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

$\{v_k, \lambda_k\}$ = 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.