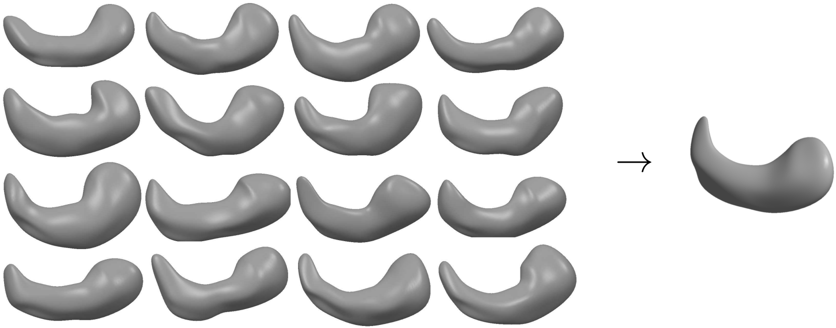
Introduction to Shape Manifolds

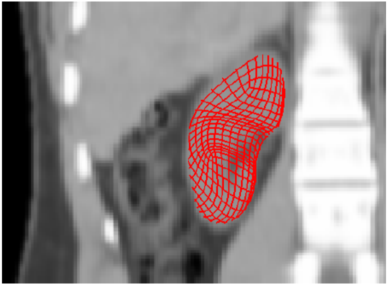
Geometry of Data

September 24, 2024

Shape Statistics: Averages

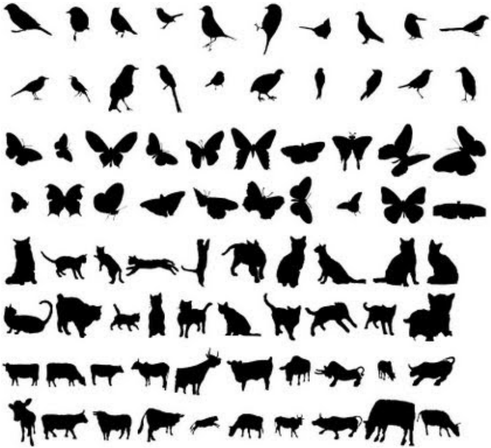


Shape Statistics: Variability



Shape priors in segmentation

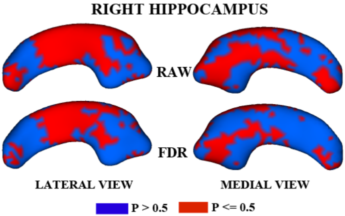
Shape Statistics: Classification

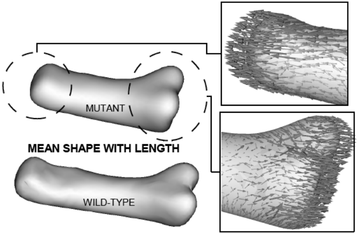


http://sites.google.com/site/xiangbai/animaldataset

Shape Statistics: Hypothesis Testing

Testing group differences





Cates, et al. IPMI 2007 and ISBI 2008

Shape Application: Bird Identification

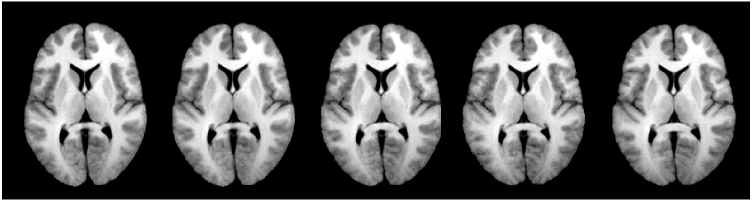
American Crow

Common Raven

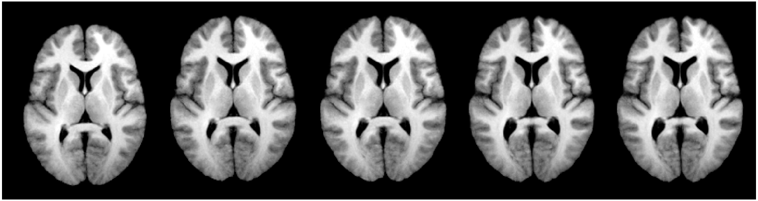
Shape Application: Box Turtles

http://www.austinsturtlepage.com/world_of_turtles/index-2.html

Shape Statistics: Regression

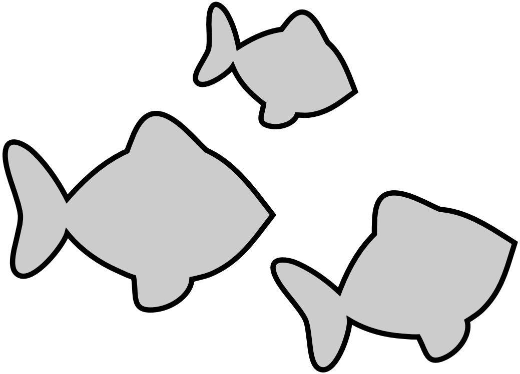


35 37 39 41 43



45 47 49 51 53

What is Shape?

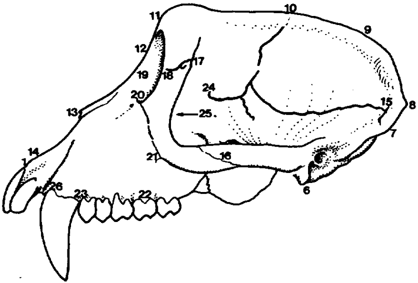


Shape is the geometry of an object modulo position, orientation, and size.

Geometry Representations

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

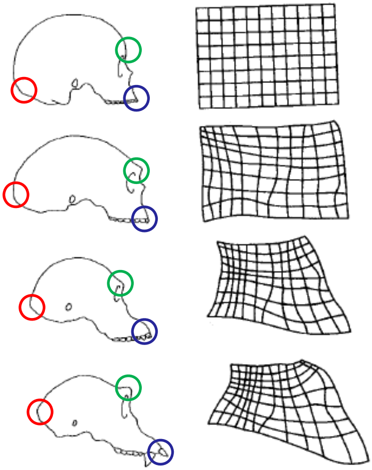
Landmarks



From Dryden & Mardia, 1998

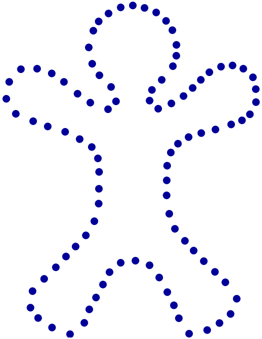
- A **landmark** is an identifiable point on an object that corresponds to matching points on similar objects.
- This may be chosen based on the application (e.g., by anatomy) or mathematically (e.g., by curvature).

Landmark Correspondence

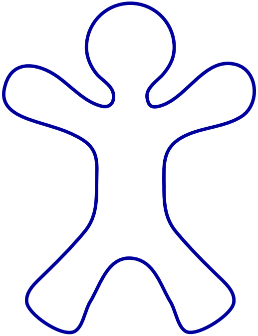


From C. Small, *The Statistical Theory of Shape*

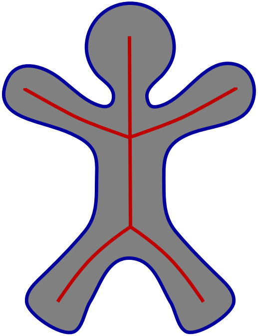
More Geometry Representations



Dense Boundary Points

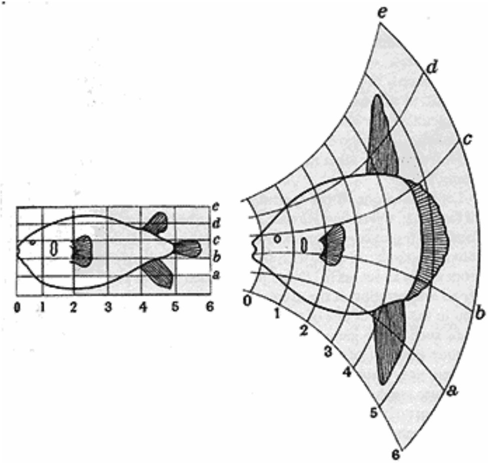


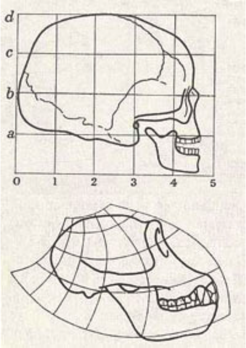
Continuous Boundary (Fourier, splines)



Medial Axis (solid interior)

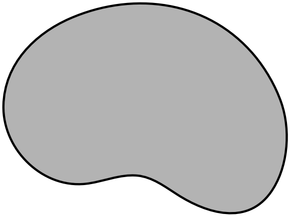
Transformation Models





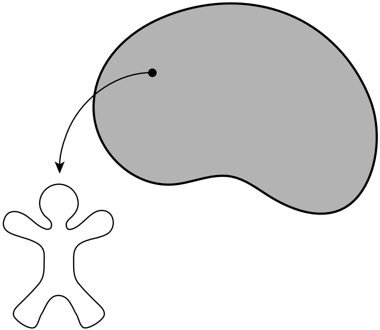
From D’Arcy Thompson, *On Growth and Form*, 1917.

Shape Spaces



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

Shape Spaces



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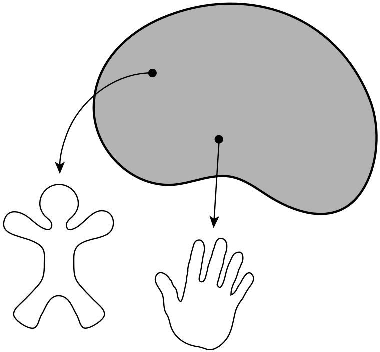

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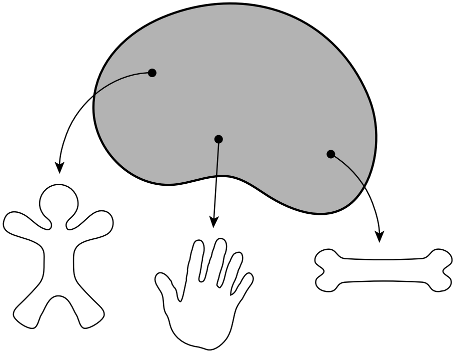

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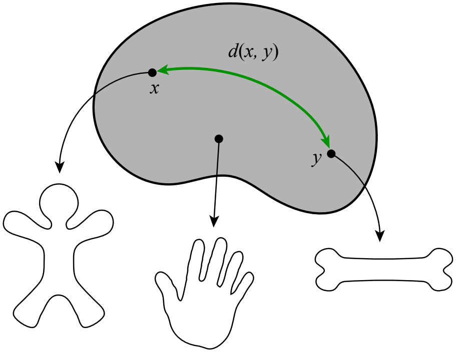
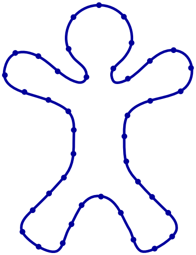


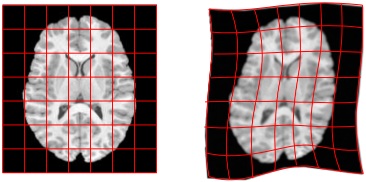
A metric space structure provides a comparison between two shapes.

Examples: Shape Spaces

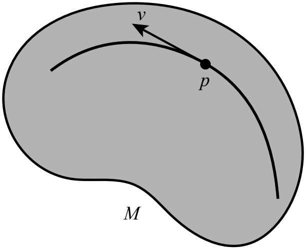
Kendall's Shape Space



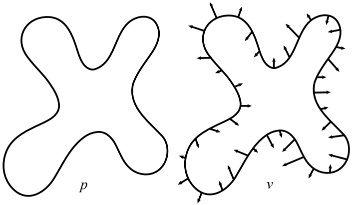
Space of Diffeomorphisms



Tangent Spaces

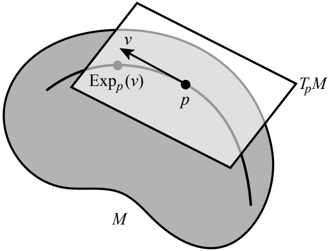


Infinitesimal change in shape:



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

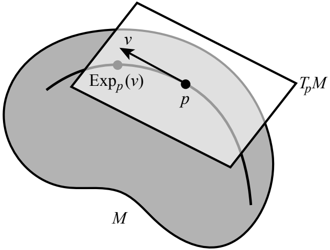
The Exponential Map



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

- 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 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**:

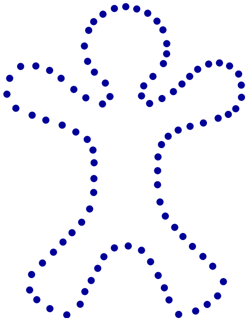
- Reflexive: $x_1 \sim x_1$
- Symmetric: $x_1 \sim x_2$ implies $x_2 \sim x_1$
- Transitive: $x_1 \sim x_2$ and $x_2 \sim x_3$ imply $x_1 \sim x_3$

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**.

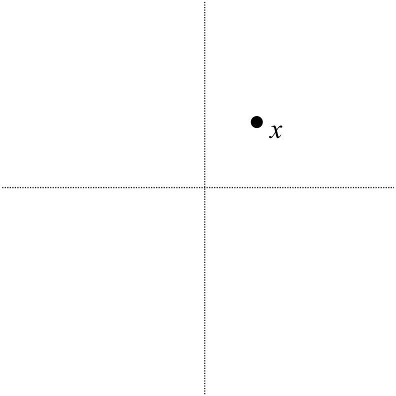
Kendall's Shape Space



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

Quotient Spaces

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



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

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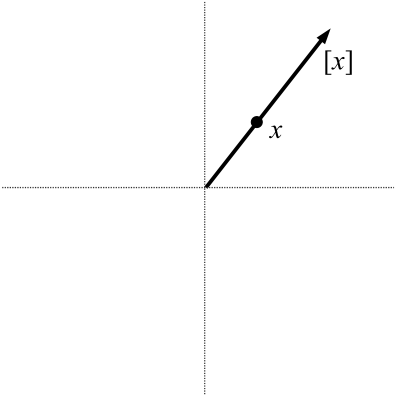

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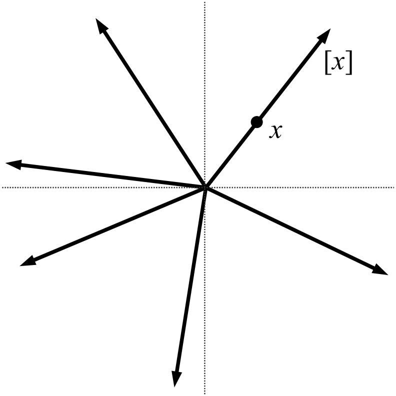

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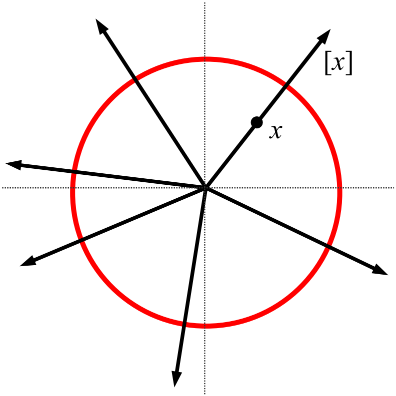

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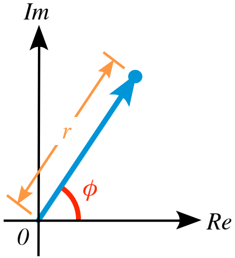
Constructing Kendall's Shape Space

- 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.

Historical Side Note

The history of Euler's formula: $e^{i\theta} = \cos\theta + i\sin\theta$

Video:

`https://www.youtube.com/watch?v=f8CXG7dS-D0`

Reading:

`http://eulerarchive.maa.org/hedi/HEDI-2007-08.pdf`

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

$$R^* = UV^T$$

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

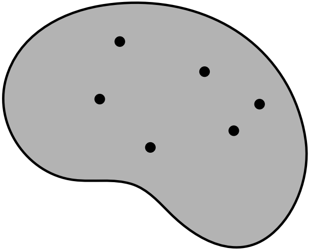
The gradient of the Riemannian distance function is

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

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

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

Computing Means



Gradient Descent Algorithm:

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

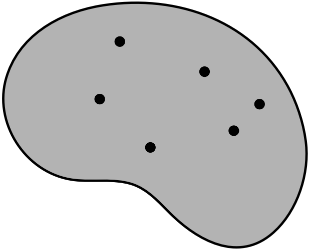
$\mu_0 = \mathbf{x}_1$

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



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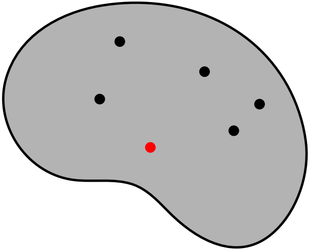

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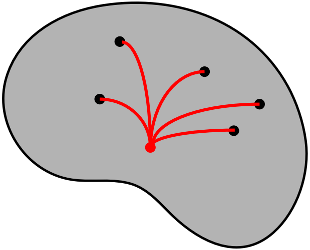

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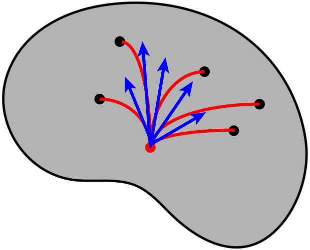

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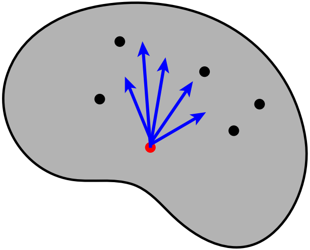

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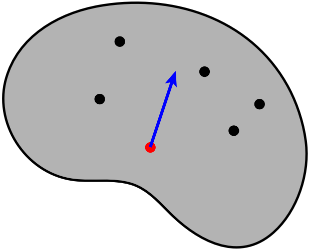

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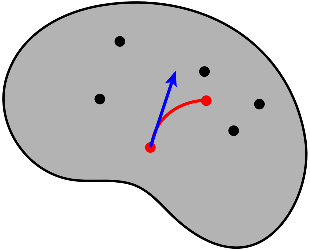

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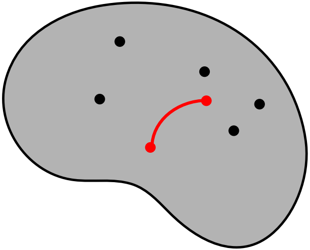

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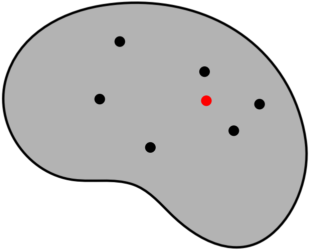

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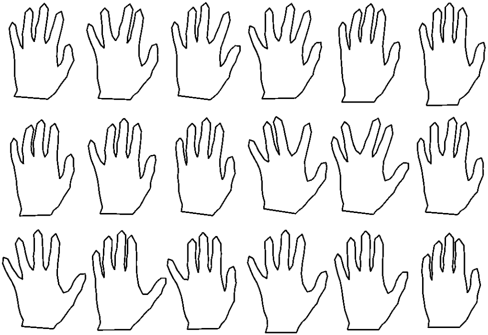
Example of Mean on Kendall Shape Space



Hand data from Tim Cootes

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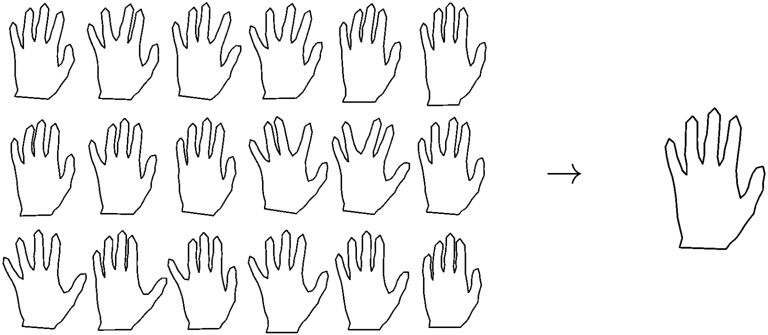
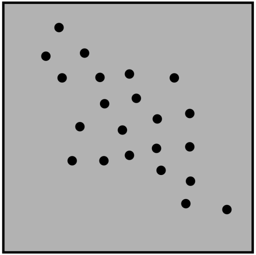


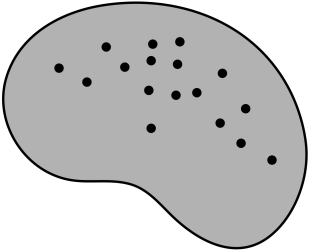
Hand data from Tim Cootes

Principal Geodesic Analysis

Linear Statistics (PCA)

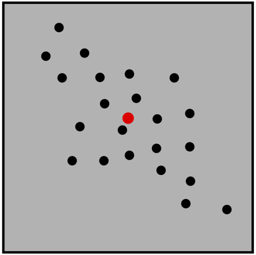


Curved Statistics (PGA)

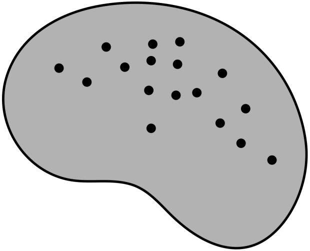


Principal Geodesic Analysis

Linear Statistics (PCA)



Curved Statistics (PGA)



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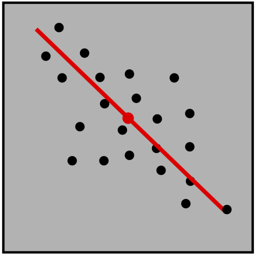

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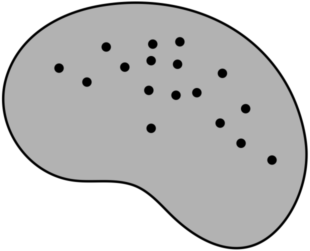

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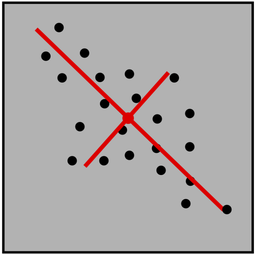

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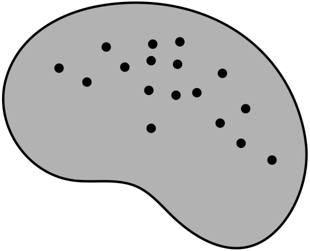

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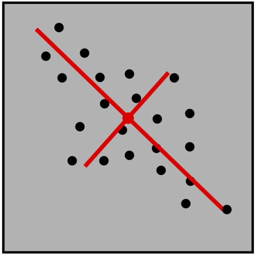
Linear Statistics (PCA)



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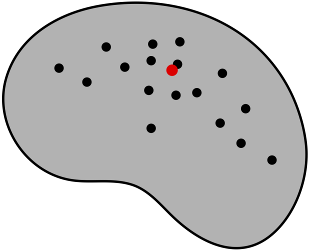
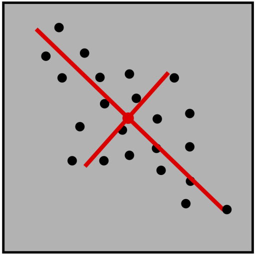


Principal Geodesic Analysis

Linear Statistics (PCA)



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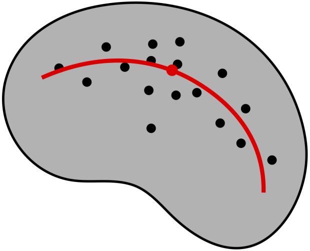
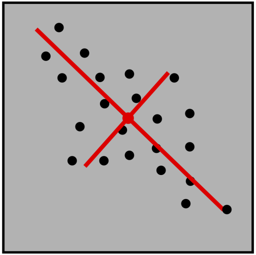


Principal Geodesic Analysis

Linear Statistics (PCA)



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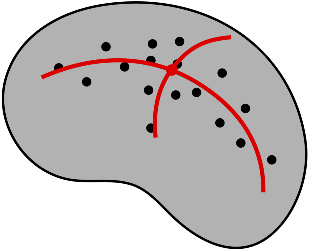

PGA of Kidney

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

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.