Statistics on Riemannian Manifolds

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Manifold Data

“Learned” Manifolds

“Known” Manifolds

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- Raw data lies in Euclidean space
- Manifold + Noise

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“Known” Manifolds

- Raw data lies in a manifold
- Typically given by some constraints on data

Manifold Data in Vision and Imaging

- Directional data

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- Transformation groups (rotations, projective, affine)

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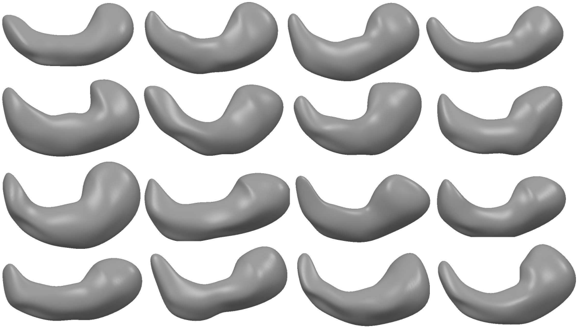
- Diffusion tensors, structure tensors
- Diffeomorphisms (for deformable atlas building)

Manifold Statistics: Averages



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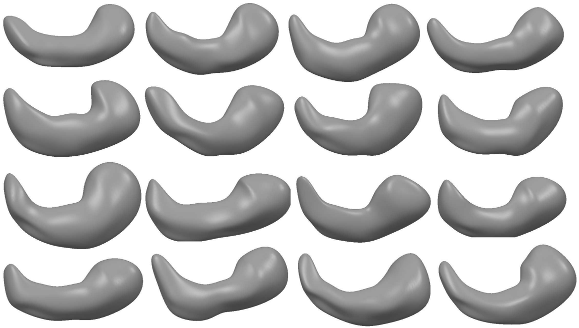

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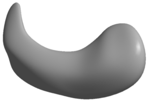
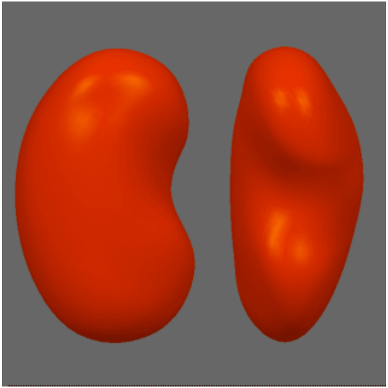
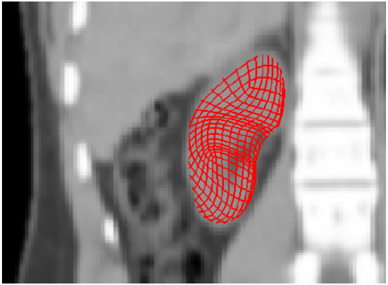


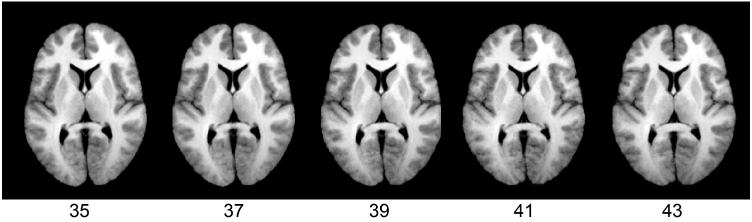
Manifold Statistics: Variability

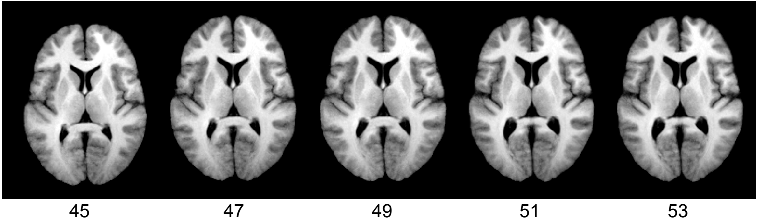




Shape priors in segmentation

Manifold Statistics: Regression





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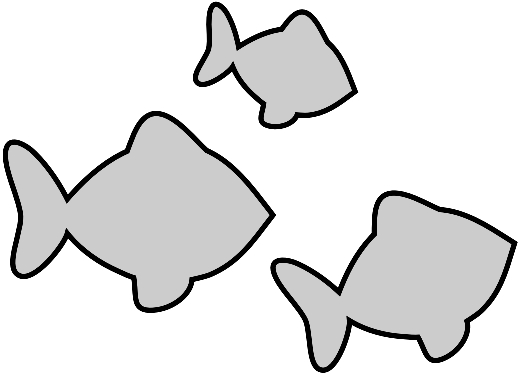

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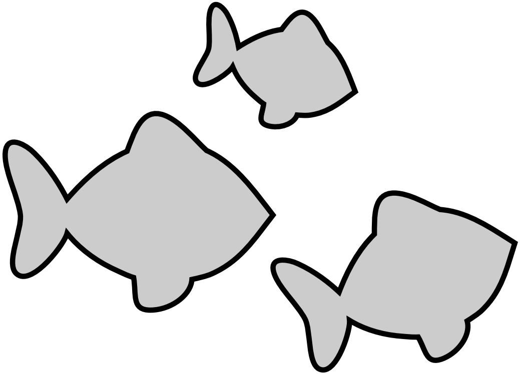
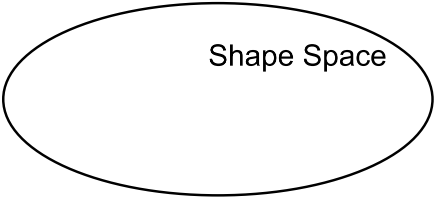


Shape is the geometry of an object modulo position, orientation, and size.

Shape Representations

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

Shape Analysis



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

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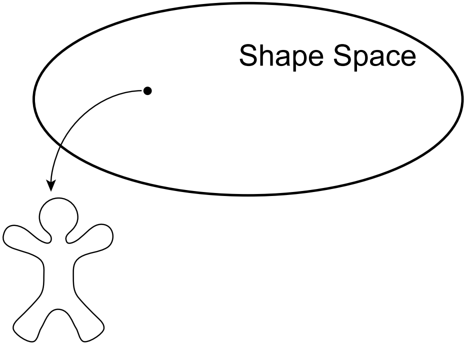

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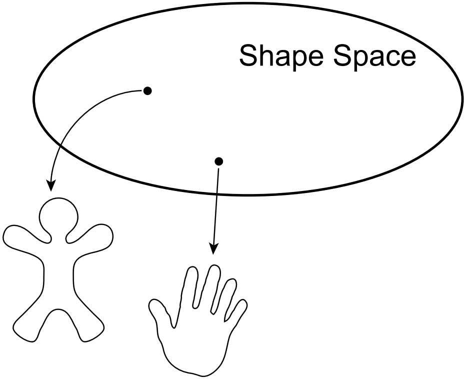

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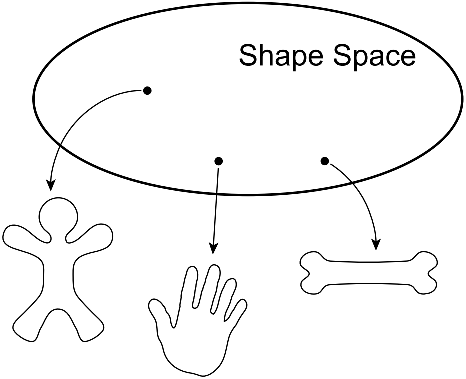

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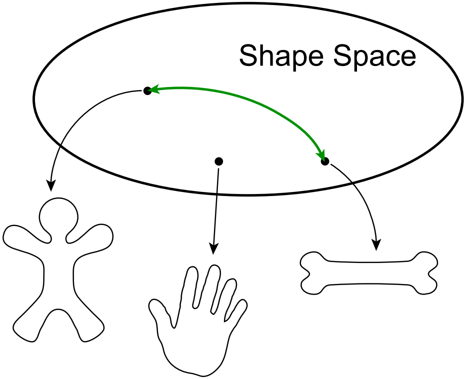
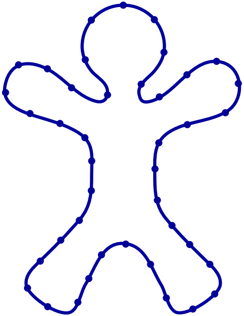


A metric space structure provides a comparison between two shapes.

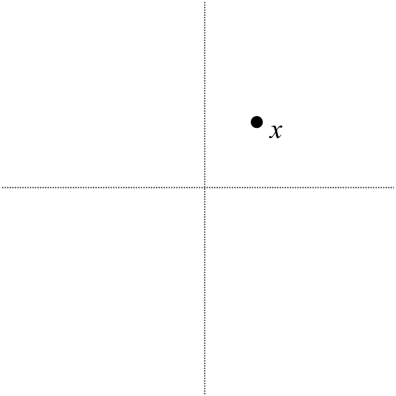
Kendall's Shape Space



- 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 $\mathbb{R}^2$?



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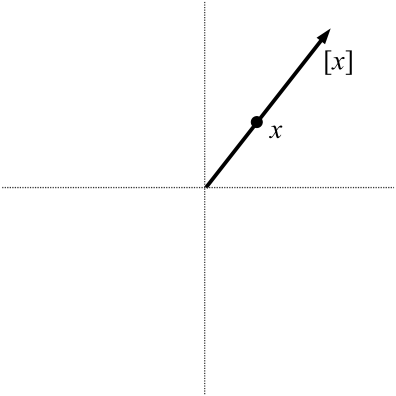

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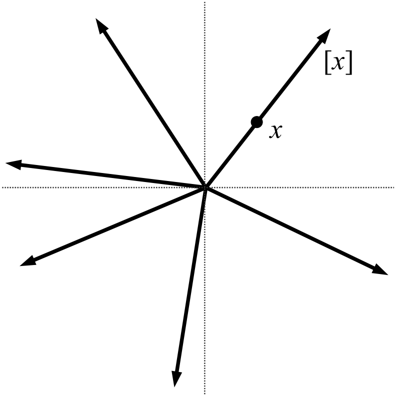

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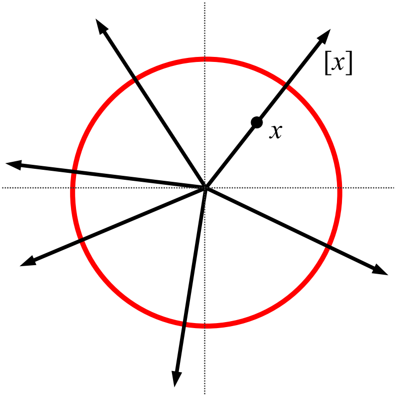

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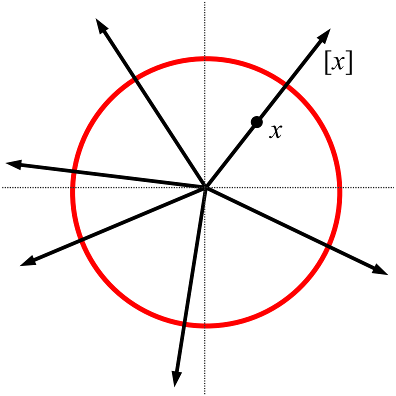

Notation: $[x] \in \mathbb{R}^2/\mathbb{R}^+$

Constructing Kendall's Shape Space

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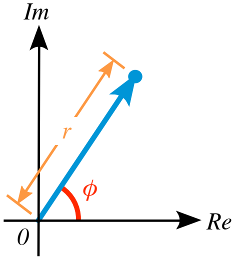
- Removing **translation** leaves us with $\mathbb{C}^{k-1}$.
- How to remove **scaling** and **rotation**?

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.

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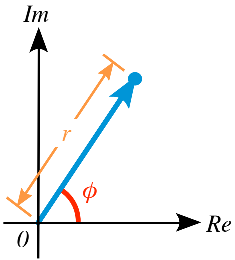

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Complex Multiplication:

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

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

Removing Scale and Translation

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.

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

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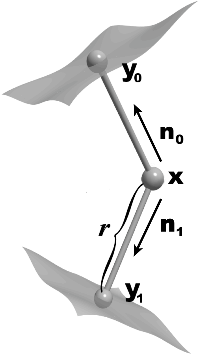
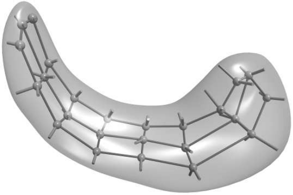
This gives complex projective space $\mathbb{CP}^{k-2}$ – much like the sphere comes from equivalence classes of scalar multiplication in $\mathbb{R}^n$.

The M-rep Shape Space





Medial Atom:

$$\mathbf{m} = \{\mathbf{x}, r, \mathbf{n}_0, \mathbf{n}_1\} \in \mathcal{M}(1)$$

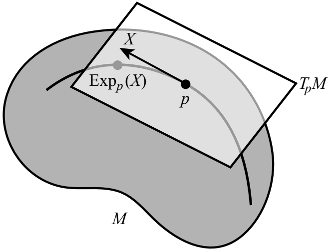
$$\mathcal{M}(1) = \mathbb{R}^3 \times \mathbb{R}^+ \times S^2 \times S^2$$

M-rep Model with n atoms:

$$\mathbf{M} \in \mathcal{M}(n) = \mathcal{M}(1)^n$$

Shape change in terms of local translation, bending, & widening.

The Exponential and Log Maps



- The exponential map takes tangent vectors to points along geodesics.
- The length of the tangent vector equals the length along the geodesic segment.
- Its inverse is the log map – it gives distance between points: $d(p, q) = \| \mathrm{Log}_p(q) \|$.

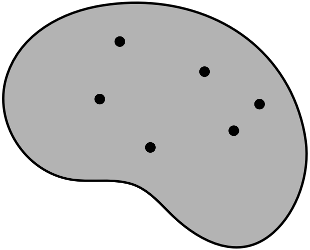
Intrinsic Means (Fréchet)

The *intrinsic mean* of a collection of points $x_1, \ldots, x_N$ on a Riemannian manifold M is

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

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

Computing Means



Gradient Descent Algorithm:

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

$\mu_0 = \mathbf{x}_1$

Repeat:

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

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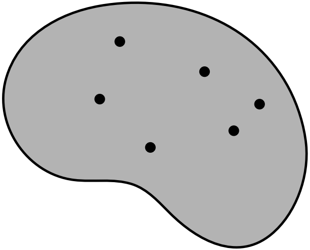

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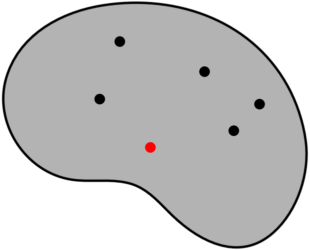

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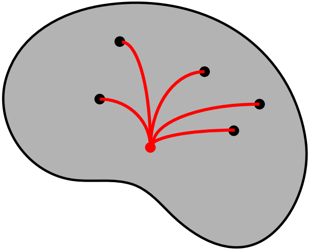

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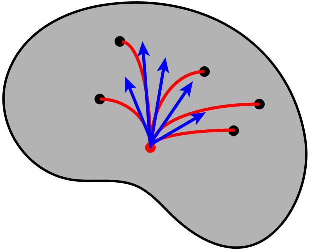

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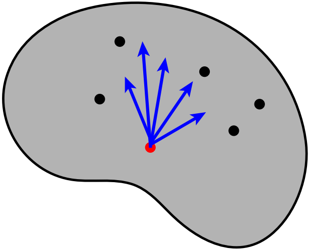

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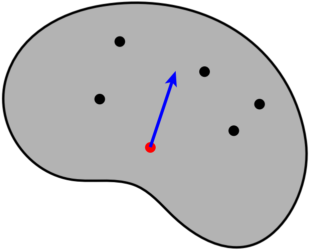

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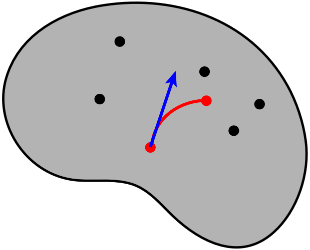

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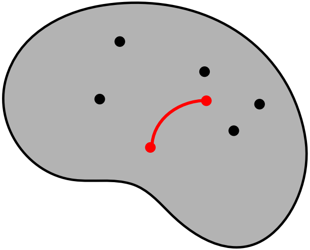

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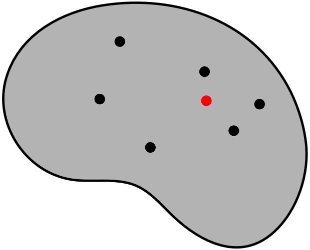

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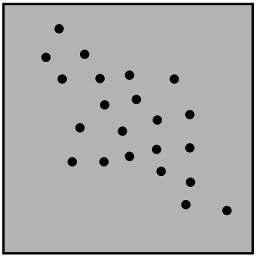

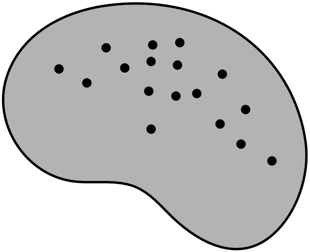

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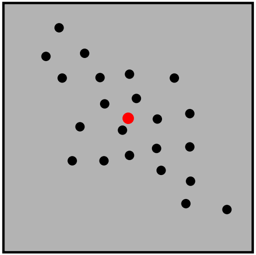
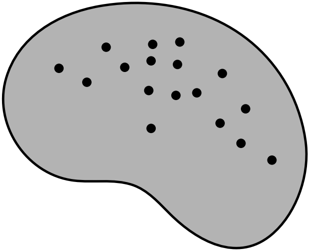
Linear Statistics (PCA)



Curved Statistics (PGA)



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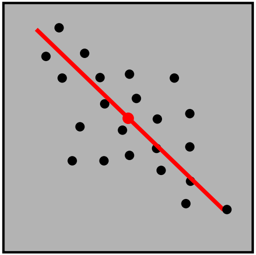

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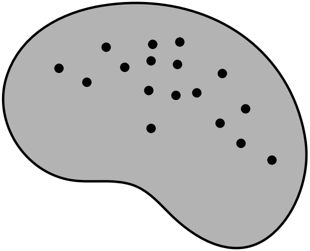

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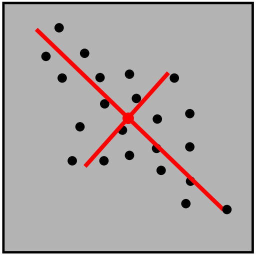

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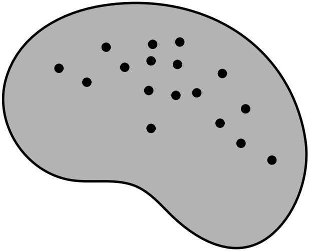

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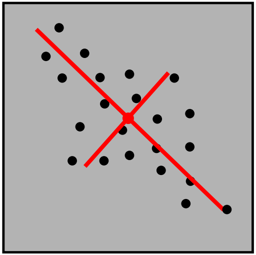

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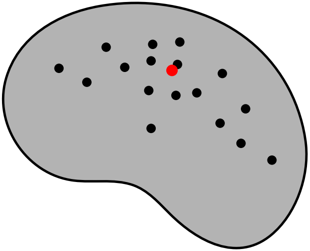

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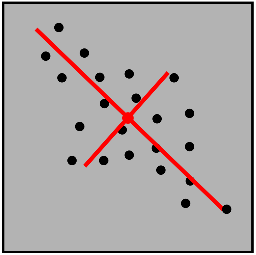

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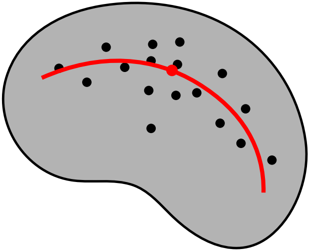

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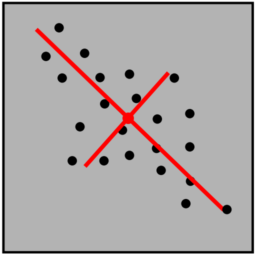
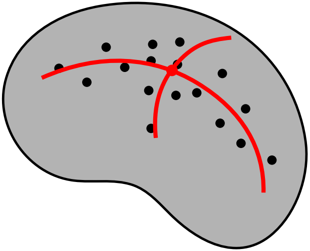
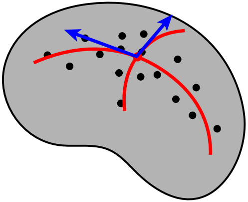


Curved Statistics (PGA)



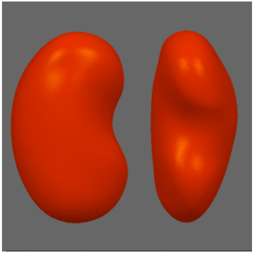
Computing PGA



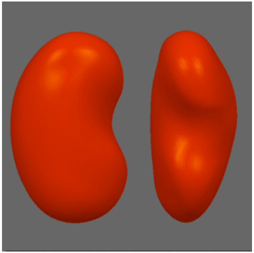
- Find nested linear subspaces $V_k \subset T_pM$ such that $\mathrm{Exp}_\mu(V_k)$ maximizes variance of projected data.
- First-order approximation: PCA in tangent space of sample covariance matrix,

$$S = \frac{1}{N-1} \sum_{i=1}^{N} \mathrm{Log}_\mu(x_i)\, \mathrm{Log}_\mu(x_i)^T$$

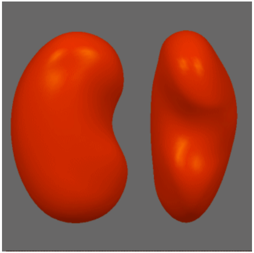
PGA of Kidney



Mode 1



Mode 2



Mode 3

Robust Statistics: Motivation

- The mean is overly influenced by outliers due to sum-of-squares.
- Robust statistical description of shape or other manifold data.
- Deal with outliers due to imaging noise or data corruption.
- Misdiagnosis, segmentation error, or outlier in a population study.

Mean vs. Median in $\mathbb{R}^n$

Mean: least-squares problem

$$\mu = \arg\min_{x \in \mathbb{R}^n} \sum \|x - x_i\|^2$$

Closed-form solution (arithmetic average)

Mean vs. Median in $\mathbb{R}^n$

Mean: least-squares problem

$$\mu = \arg\min_{x \in \mathbb{R}^n} \sum \|x - x_i\|^2$$

Closed-form solution (arithmetic average)

Geometric Median, or Fermat-Weber Point:

$$m = \arg\min_{x \in \mathbb{R}^n} \sum \|x - x_i\|$$

No closed-form solution

Weiszfeld Algorithm in $\mathbb{R}^n$

- Gradient descent on sum-of-distance:

$$m_{k+1} = m_k - \alpha G_k,$$
$$G_k = \sum_{i \in I_k} \frac{m_k - x_i}{\|x_i - m_k\|} \Bigg/ \left(\sum_{i \in I_k} \|x_i - m_k\|^{-1} \right)$$

- Step size: $0 < \alpha \leq 2$
- Exclude singular points: $I_k = \{i : m_k \neq x_i\}$
- Weiszfeld (1937), Ostresh (1978)

Geometric Median on a Manifold

The geometric median of data $x_i \in M$ is the point that minimizes the sum of geodesic distances:

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

Fletcher, et al. CVPR 2008 and NeuroImage 2009.

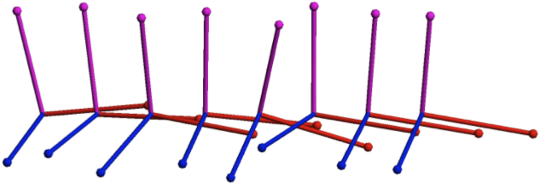
Weiszfeld Algorithm for Manifolds

Gradient descent:

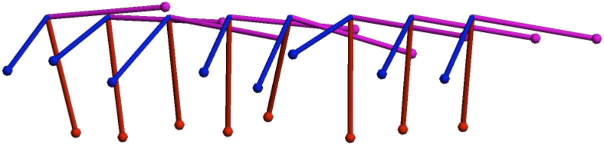
$$
\begin{aligned}
m_{k+1} &= \mathrm{Exp}_{m_k}(\alpha v_k), \\
v_k &= \sum_{i \in I_k} \frac{\mathrm{Log}_{m_k}(x_i)}{d(m_k, x_i)} \Bigg/ \left(\sum_{i \in I_k} d(m_k, x_i)^{-1} \right)
\end{aligned}
$$

Example: Rotations

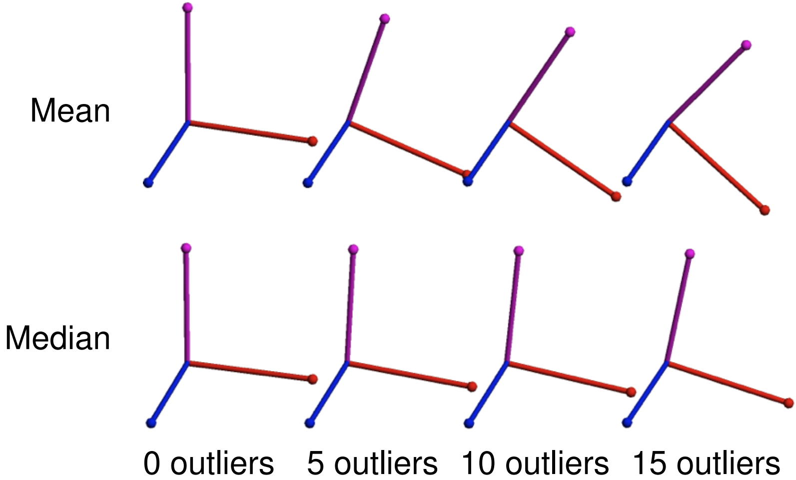
Input data: 20 random rotations



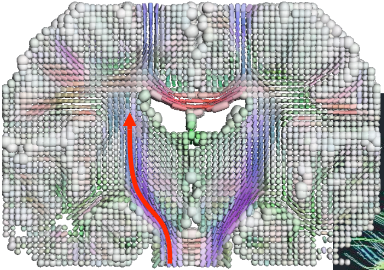
Outlier set: random, rotated 90°

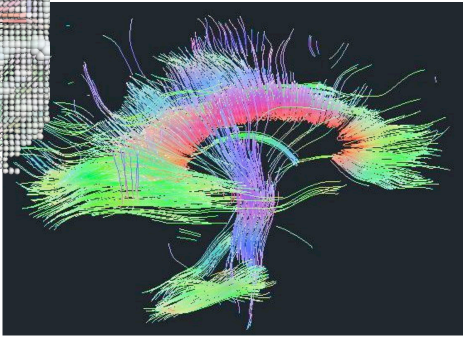


Example: Rotations



Application: Diffusion Tensor MRI





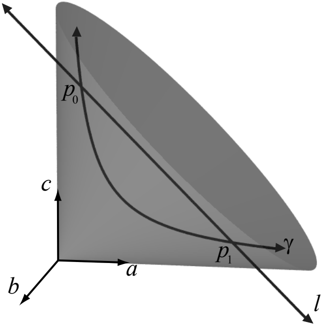
Space of Positive-Definite Tensors

- Positive-definite, symmetric matrices

$$\mathrm{PD}(n) = \mathrm{GL}^+(n)/\mathrm{SO}(n)$$

- Riemannian manifold with nonpositive curvature
- Applications:
  - Diffusion tensor MRI: Fletcher (2004), Pennec (2004)
  - Structure tensor: Rathi (2007)
  - Bookstein's simplex shape space (1986)

Example: $\mathrm{PD}(2)$



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

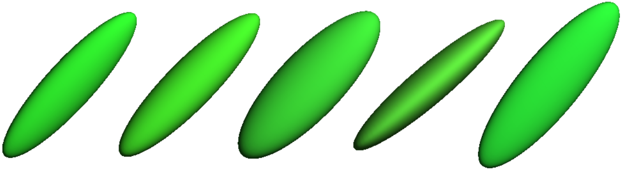
$$A = \begin{pmatrix} a & b \\ b & c \end{pmatrix},$$

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

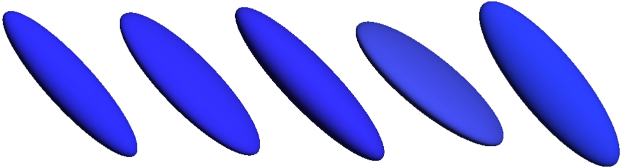
Similar situation for $\mathrm{PD}(3)$ (6-dimensional).

Example: Tensors

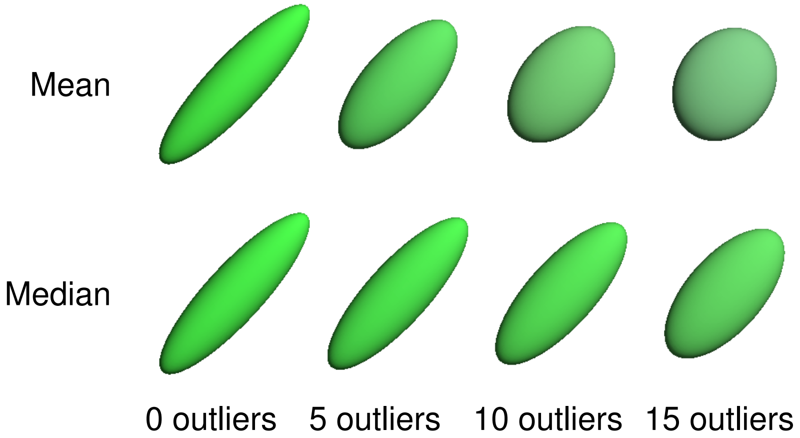
Input data: 20 random tensors



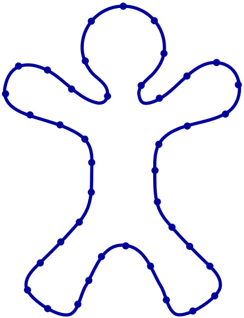
Outlier set: random, rotated 90°



Example: Tensors

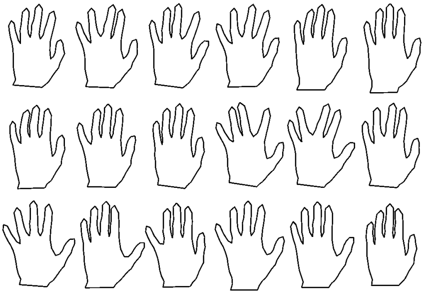


Kendall's Shape Space

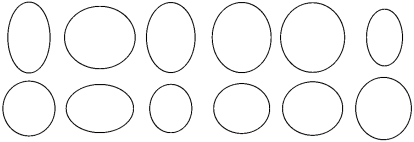


- Define object with k points.
- Represent as a vector in $\mathbb{R}^{2k}$.
- Remove translation, rotation, and scale.
- End up with complex projective space, $\mathbb{CP}^{k-2}$.

Example on Kendall Shape Spaces



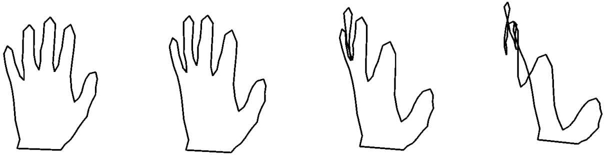
Hand shapes



Outliers

Example on Kendall Shape Spaces

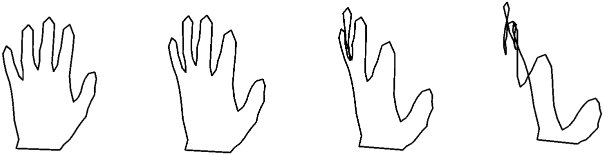
Mean:



Outliers: 0 2 6 12

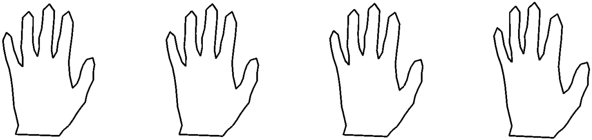
Example on Kendall Shape Spaces

Mean:



Outliers: 0 2 6 12

Median:



Outliers: 0 2 6 12

Image Metamorphosis

- Metric between images
- Includes both deformation and intensity change

$$U(v_t, I_t) = \int_0^1 \|v_t\|_V^2 \, dt \;+\; \frac{1}{\sigma^2} \int_0^1 \left\| \frac{dI_t}{dt} + \langle \nabla I_t, v_t \rangle \right\|_{L^2}^2 dt$$

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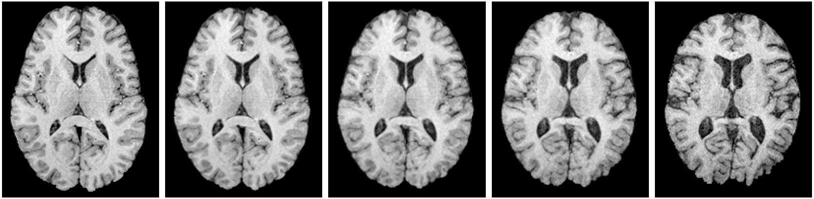
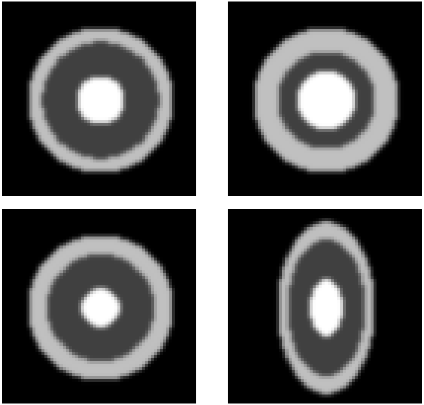
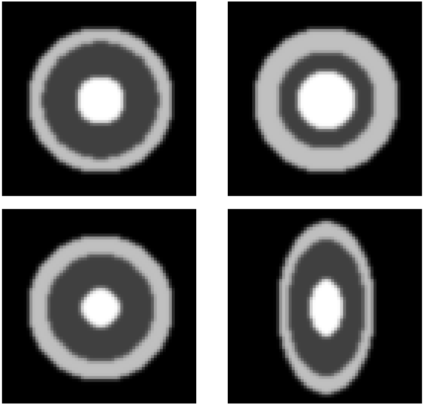


Example: Metamorphosis

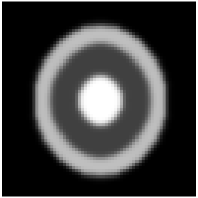


Input Data

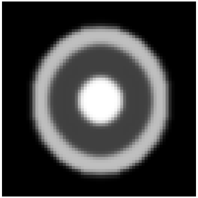
Example: Metamorphosis



Input Data

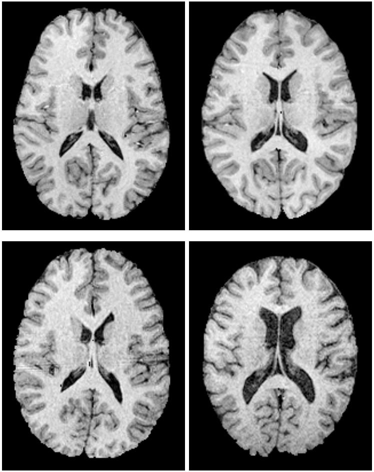


Mean
ratio = 1.13

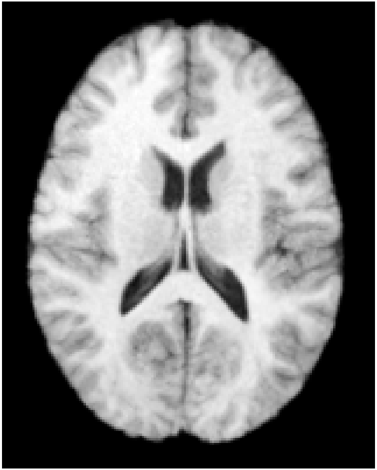


Median
ratio = 1.04

Example: Metamorphosis



Input Data



Median Atlas

Preliminaries

- $x_i \in U \subset M$, U is a convex subset
- $\mathrm{diam}(U) = \max_{x,y \in U} d(x, y)$

Existence and Uniqueness

Theorem. *The weighted geometric median exists and is unique if*

1. *the sectional curvatures of* M *are bounded above by* $\Delta > 0$ *and* $\mathrm{diam}(U) < \pi/(2\sqrt{\Delta})$, *or*
2. *the sectional curvatures of* M *are nonpositive.*

Existence and Uniqueness

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1. *the sectional curvatures of M are bounded above by $\Delta > 0$ and $\mathrm{diam}(U) < \pi/(2\sqrt{\Delta})$, or*
2. *the sectional curvatures of M are nonpositive.*

Proof is by showing the convexity of geodesic distance.

Identical conditions to ensure the mean (Karcher).

Robustness

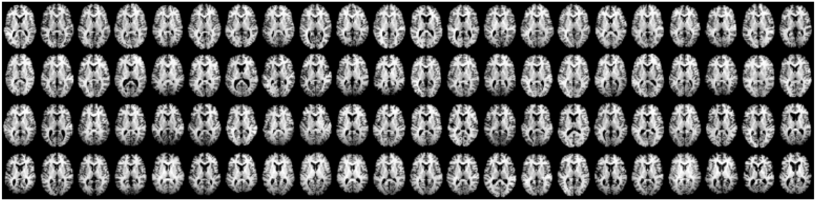
- Breakdown point: percentage of points that can be moved to infinity before statistic goes to infinity
- Euclidean mean: 0%
- Euclidean geometric median: 50%
- Same result holds for noncompact manifolds
- Does not make sense for compact manifolds

Convergence Theorem for Manifold Weiszfeld Algorithm

Theorem. *If the sectional curvatures of* M *are nonnegative and the existence/uniqueness conditions are satisfied, then* $\lim_{k\to\infty} m_k = m$ *for* $0 < \alpha \leq 2$*.*

Describing Shape Change

- How does shape change over time?
- Changes due to growth, aging, disease, etc.
- Example: 100 healthy subjects, 20–80 yrs. old



- We need regression of shape!

Regression Analysis

- Describe relationship between a dependent random variable Y to an independent random variable T.
- Given observations (T_i, Y_i), find regression function: $Y = f(T)$.
- Often phrased as conditional expectation $E[Y|T = t] = f(t)$.
- Parametric (e.g., linear) or nonparametric (e.g., kernel).

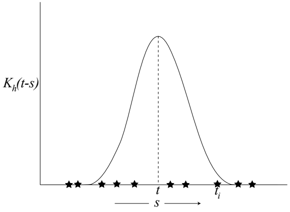
Kernel Regression (Nadaraya-Watson)

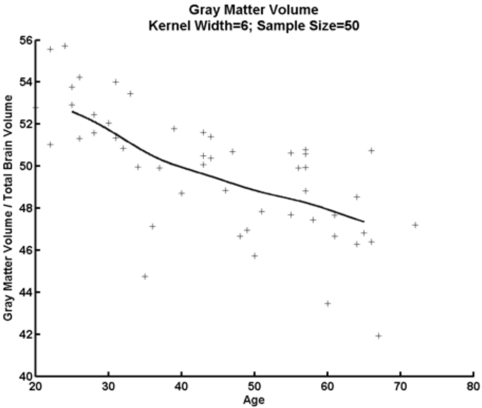
Define regression function through weighted averaging:

$$f(t) = \sum_{i=1}^{N} w_i(t) Y_i$$

$$w_i(t) = \frac{K_h(t - T_i)}{\sum_{i=1}^{N} K_h(t - T_i)}$$

Example: Gray Matter Volume

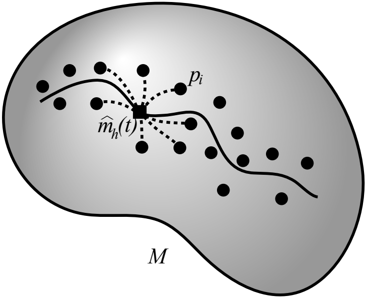




$$w_i(t) = \frac{K_h(t - T_i)}{\sum_{i=1}^{N} K_h(t - T_i)}$$

$$f(t) = \sum_{i=1}^{N} w_i(t) Y_i$$

Manifold Kernel Regression

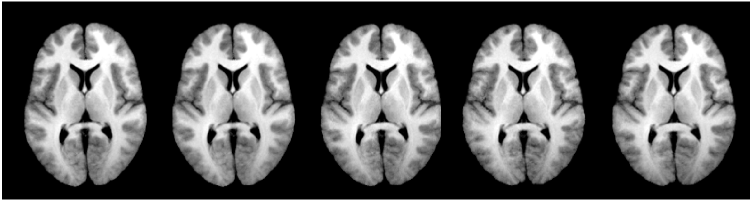


Using Fréchet weighted average:

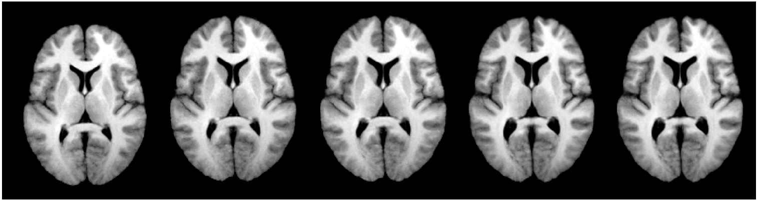
$$\hat{m}_h(t) = \arg\min_y \sum_{i=1}^{N} w_i(t) d(y, Y_i)^2$$

Davis, et al. ICCV 2007

Brain Shape Regression



35 37 39 41 43



45 47 49 51 53

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- Brad Davis (Kitware)

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