Manifold Statistics: Fréchet Mean

Geometry of Data

September 23, 2021

This lecture is about statistical analysis of data on a **known manifold**.

Such data often arises from nonlinear constraints.

For example, if your data has unit length (such as directional data), it lives on the unit sphere, S^d.

Theorem. Let $f : M \to N$ be a smooth map between two manifolds of dimension $m \geq n$. If $y \in N$ is a regular value, then the set $f^{-1}(y)$ is a smooth manifold of dimension $m - n$.

Manifold Examples

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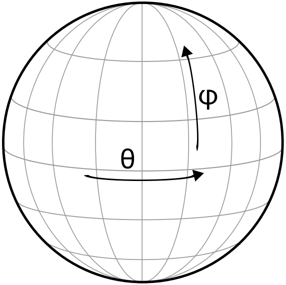
- **The Sphere:** S^d
  - Local coordinate chart for S^2:

$$(-\pi, \pi) \times (0, 2\pi) \to S^2$$

$$(\theta, \phi) \mapsto (\cos(\theta)\cos(\phi), \cos(\theta)\sin(\phi), \sin(\theta))$$



Manifold Examples: Matrix Groups

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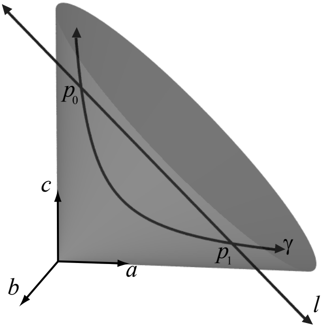
  - Open set of $\mathbb{R}^{n\times n}$
- **Special Orthogonal Group:** $\mathrm{SO}(n)$
  - Rotations of $\mathbb{R}^n$
  - All matrices $R \in \mathrm{GL}(n)$ such that $RR^T = I$ and $\det(R) = 1$

Manifold Examples: Positive-Definite Tensors



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

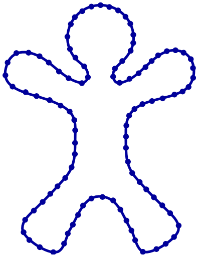
$$A = \begin{pmatrix} a & b \\ b & c \end{pmatrix},$$

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

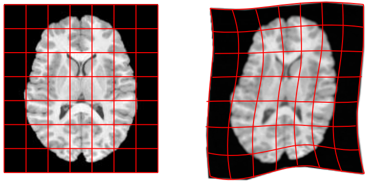
Similar situation for $\mathrm{PD}(3)$ (6-dimensional) or $\mathrm{PD}(d)$.

Manifold Examples: Shape Spaces

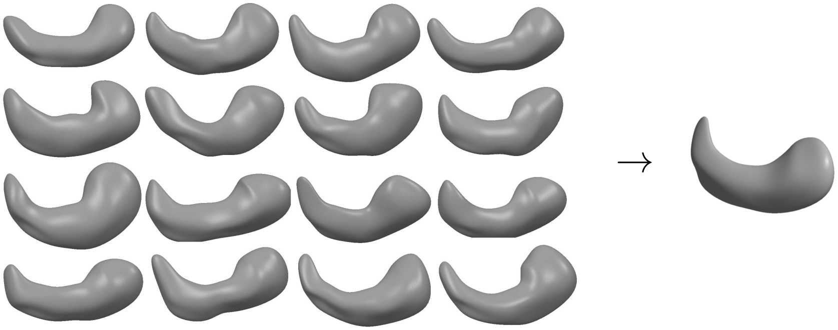
Kendall's Shape Space



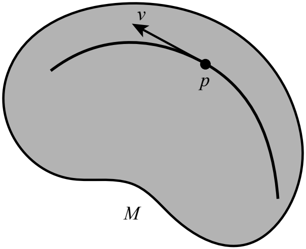
Space of Diffeomorphisms



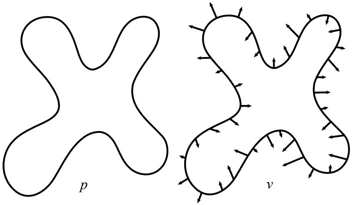
Shape Statistics: Averages



Review: Tangent Spaces



Infinitesimal change in shape:



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

Review: Riemannian Metrics

A **Riemannian metric** is a smoothly varying inner product on the tangent spaces, denoted $\langle v, w \rangle_p$ for $v, w \in T_p M$.

This metric now gives us the **norm** of a tangent vector:

$$\|v\|_p = \sqrt{\langle v, v \rangle_p}.$$

Review: Geodesics

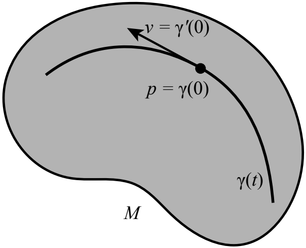
A **geodesic** is a curve $\gamma \in M$ that locally minimizes

$$E(\gamma) = \int_0^1 \|\gamma'(t)\|^2 dt.$$

Turns out it also locally minimizes arc-length,

$$L(\gamma) = \int_0^1 \|\gamma'(t)\| dt.$$

Review: Directional Derivatives



Tangent vector $v \in T_pM$ is directional derivative operator on smooth functions, $f : M \to \mathbb{R}$

Notation: $vf(p) = \frac{d}{dt} f(\gamma(t))\,|_{t=0}$

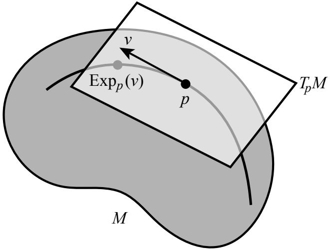
Gradient on a Manifold

Given $f : M \to \mathbb{R}$, define gradient $\operatorname{grad} f(p)$ as vector in T_pM such that:

$$vf(p) = \langle \operatorname{grad} f(p), v \rangle,$$

for all tangent vectors $v \in T_pM$.

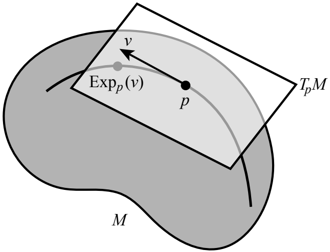
The Exponential Map



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

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

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: $d(p, q) = \| \mathrm{Log}_p(q) \|$.

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

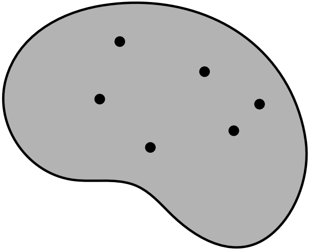
The gradient of the Riemannian distance function is

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

So, 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:

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

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

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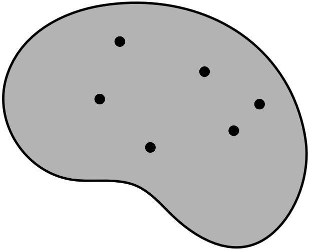

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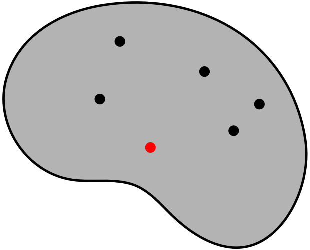

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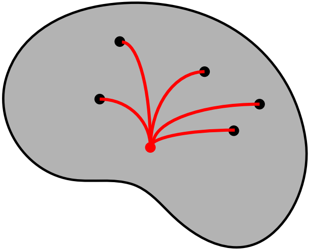

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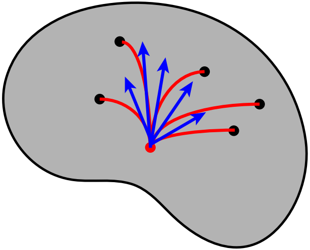

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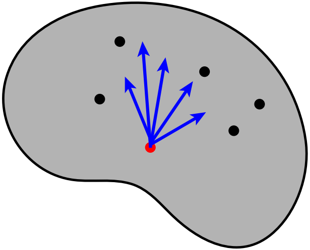

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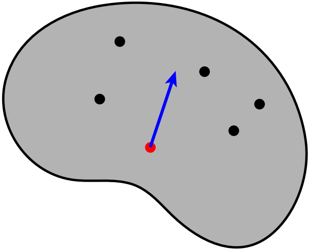

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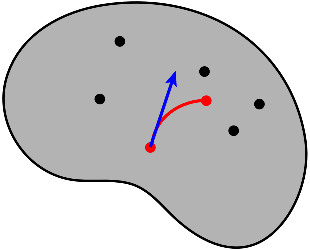

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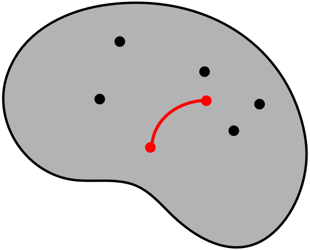

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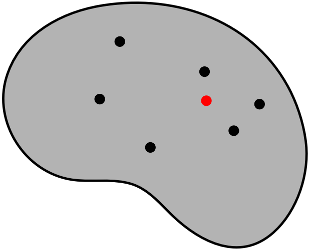

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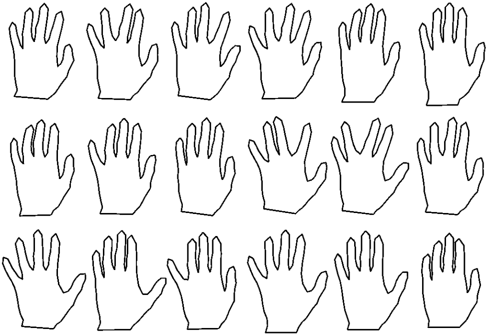
Example of Mean on Kendall Shape Space



Hand data from Tim Cootes

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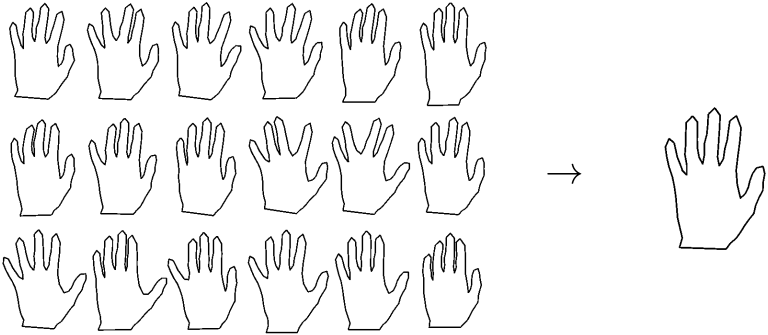

Hand data from Tim Cootes

Least Squares and Maximum Likelihood

Geometric: Least squares

$$\min_{\text{model}} \sum_{i=1}^{N} d(\text{model}, y_i)^2$$

Probabilistic: Maximum likelihood

$$\max_{\text{model}} \prod_{i=1}^{N} p(y_i; \text{model})$$

How about this "Gaussian" likelihood?

$$p(y_i; \text{model}) \propto \exp\left(-\tau d(\text{model}, y_i)^2\right)$$

A Riemannian Normal Distribution

For a simple model with Fréchet mean:

$$p(y; \mu, \tau) = \frac{1}{C(\mu, \tau)} \exp\left(-\tau d(\mu, y)^2\right)$$

Notation: $y \sim N_M(\mu, \tau^{-1})$

Problem: Normalizing constant may depend on μ:

$$\ln p(y; \mu, \tau) = -\ln C(\mu, \tau) - \tau d(\mu, y)^2$$

Note: not a problem in $\mathbb{R}^d$ because $C(\mu, \tau) \propto \tau^{-d/2}$.

Riemannian Homogeneous Spaces

Definition: A Riemannian manifold M is called a **Riemannian homogeneous space** if its isometry group G acts transitively.

Theorem: If M is a homogeneous space, the normalizing constant for a normal distribution on M does not depend on μ.

Fletcher, IJCV 2013

Examples of Homogeneous Spaces

- **Constant curvature spaces:** Euclidean spaces, spheres, hyperbolic spaces
- **Lie groups:** $\mathrm{SO}(n)$ (rotations), $\mathrm{SE}(n)$ (rigid transforms), $\mathrm{GL}(n)$ (non-singular matrices), $\mathrm{Aff}(n)$ (affine transforms), etc.
- **Stiefel manifolds:** space of orthonormal k-frames in $\mathbb{R}^n$
- **Grassmann manifolds:** space of k-dimensional subspaces in $\mathbb{R}^n$
- **Positive-definite symmetric matrices**