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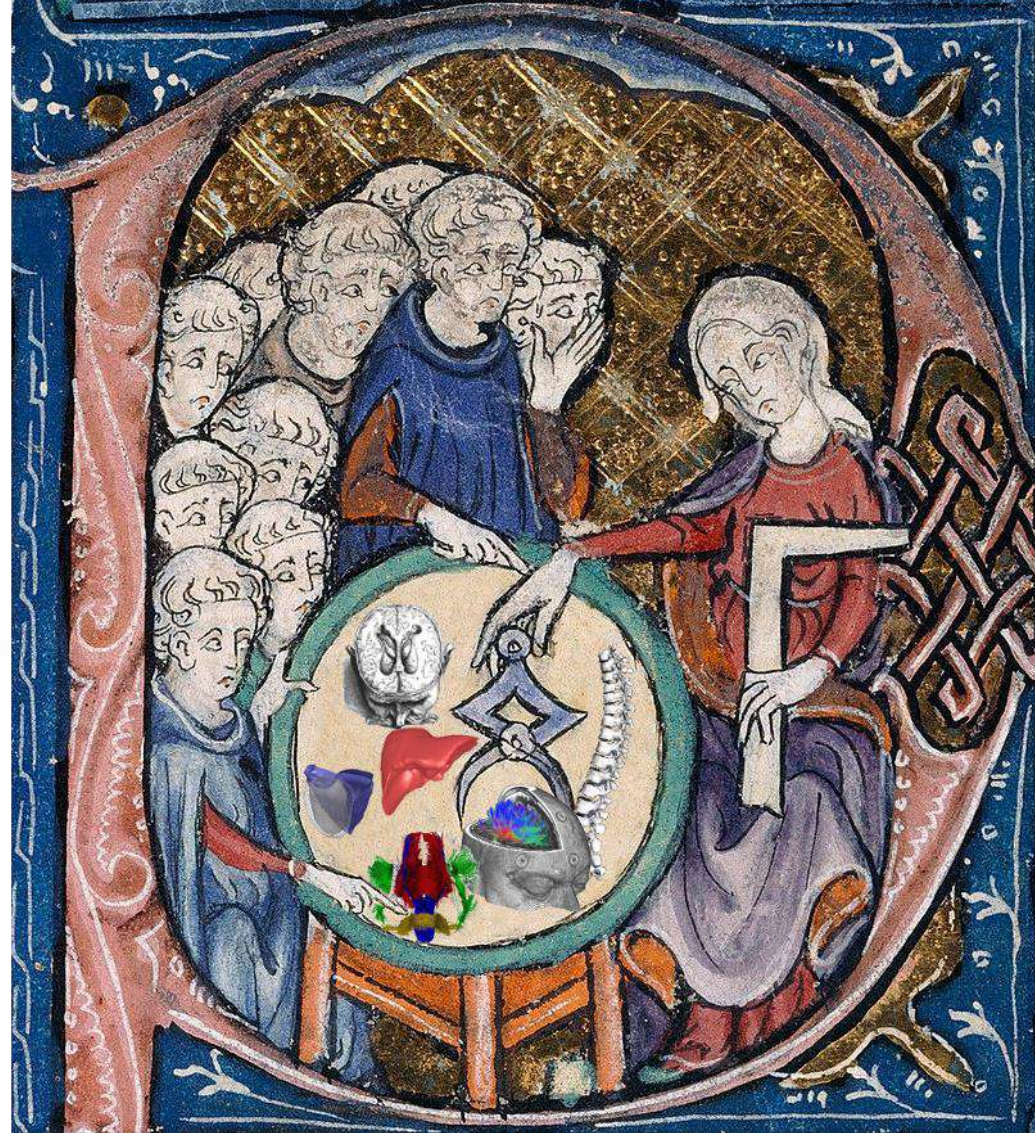
*Ecole Normale Supérieure Paris-
Saclay*

Minicourse

**Shape Spaces and
Geometric Statistics**

TGSI, Luminy 31-08-2017

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Shape Spaces and Geometric Statistics

Shape spaces: quotient or not quotient?

Geometric statistics

- **Simple statistics on Riemannian manifolds**
- Subspaces for PCA in manifolds
- Perspectives, open problems

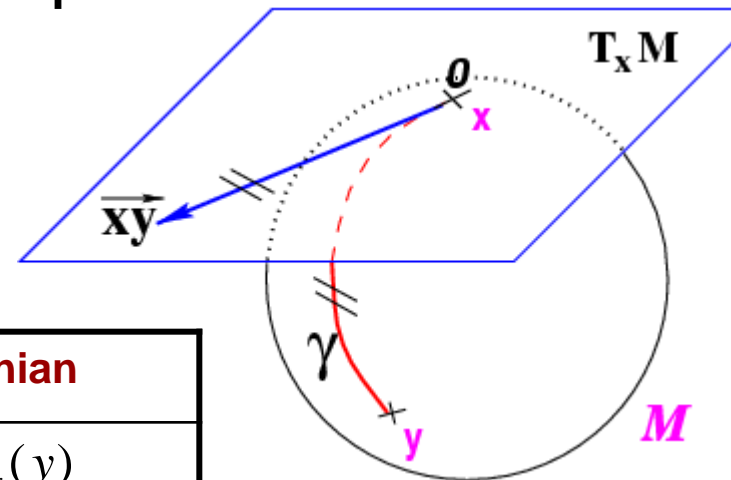
Computing in Riemannian Manifolds

Exponential map (Normal coordinate system):

- $\text{Exp}_x(\mathbf{v})$ = geodesic shooting at x parameterized by the initial tangent vector \mathbf{v}
- $\text{Log}_x(\mathbf{y})$ = development of the manifold in the tangent space along geodesics
 - Geodesics = straight lines with Euclidean distance
 - Local \rightarrow global domain: star-shaped, limited by the cut-locus
 - Covers all the manifold if **geodesically complete**

Reformulate algorithms with exp_x and log_x

Vector \rightarrow Bi-point (no more equivalence classes)



Operation	Euclidean space	Riemannian
Subtraction	$\overrightarrow{xy} = y - x$	$\overrightarrow{xy} = \text{log}_x(y)$
Addition	$y = x + \overrightarrow{xy}$	$y = \text{exp}_x(\overrightarrow{xy})$
Distance	$\text{dist}(x, y) = \ y - x\ $	$\text{dist}(x, y) = \ \overrightarrow{xy}\ _x$
Gradient descent	$x_{t+\varepsilon} = x_t - \varepsilon \nabla C(x_t)$	$x_{t+\varepsilon} = \text{exp}_{x_t}(-\varepsilon \nabla C(x_t))$

Random variable in a Riemannian Manifold

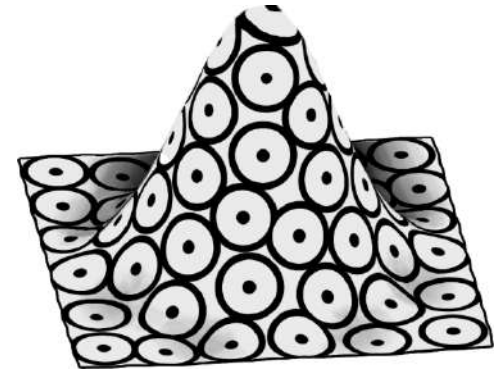
Intrinsic pdf of \mathbf{x}

- For every set H

$$P(\mathbf{x} \in H) = \int_H p(y) dM(y)$$

- ~~□ Lebesgue's measure~~

→ Uniform Riemannian Measure $dM(y) = \sqrt{\det(G(y))} dy$



Expectation of an observable in M

- $E_{\mathbf{x}}[\phi] = \int_M \phi(y) p(y) dM(y)$
- $\phi = dist^2$ (variance) : $E_{\mathbf{x}}[dist(., y)^2] = \int_M dist(y, z)^2 p(z) dM(z)$
- $\phi = \log(p)$ (information) : $E_{\mathbf{x}}[\log(p)] = \int_M p(y) \log(p(y)) dM(y)$
- ~~□ $\phi = x$ (mean) : $E_{\mathbf{x}}[\mathbf{x}] = \int_M y p(y) dM(y)$~~

Statistical tools: Moments

Frechet mean [1944] minimize the variance

$$\square \sigma^2(x) = \int_M \text{dist}^2(x, z) p(z) dM(z)$$

□ Tensor moments of a random point with density p

• $\mathfrak{M}_1(x) = \int_M \overrightarrow{xz} p(z) dM(z)$ Tangent mean field

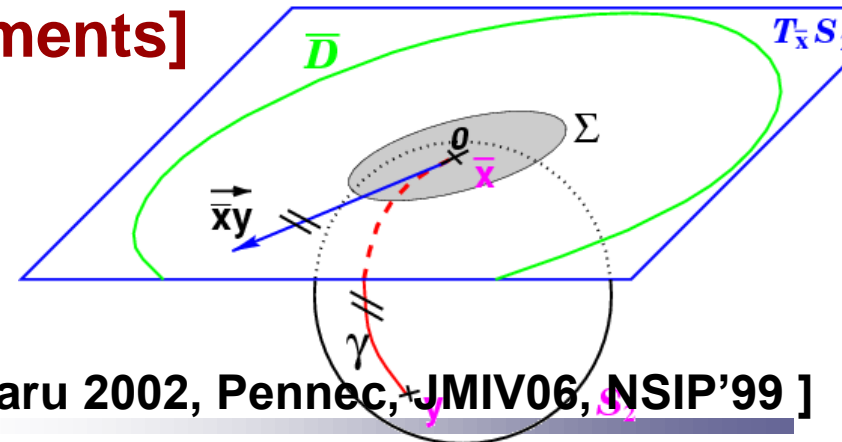
• $\mathfrak{M}_2(x) = \int_M \overrightarrow{xz} \otimes \overrightarrow{xz} p(z) dM(z)$ Covariance field

Exponential barycenters are critical pts of variance ($P(C) = 0$)

$$\square \mathfrak{M}_1(\bar{x}) = \int_M \overrightarrow{\bar{x}z} p(z) dM(z) = 0 \quad (\text{implicit definition of } \bar{x})$$

Covariance [and higher order moments]

$$\square \mathfrak{M}_2(\bar{x}) = \int_M \overrightarrow{\bar{x}z} \otimes \overrightarrow{\bar{x}z} p(z) dM(z)$$



[Oller & Corcuera 95, Battacharya & Patrangenaru 2002, Pennec, JMIV06, NSIP'99]

Riemannian center of mass, Fréchet or Karcher mean?

A naming dispute [Karcher 2014]

- For simply connected Riemannian manifolds of non-positive curvature, the minimum of the variance is unique [Cartan 1929]
- Exponential barycenter called THE Riemannian center of mass (under some uniqueness assumptions) [Groove & Karcher 1973-1976]
- Current conventions in geometric statistics:
[Fréchet 1944] set of **global** minima / [Karcher 1977] = set of **local** minima
[Emery 1991, Oller & Corcuera 1995] Exp. barycenters = set of critical points

Existence and uniqueness (extensions to p-means)

[Karcher 77 / Buser & Karcher 1981 / Kendall 90 / Afsari 10 / Le 11]

- Support of distribution in a regular geodesic ball $U(r)$ with radius $r < r^* = \frac{1}{2} \min(\text{inj}(M), \pi/\sqrt{\kappa})$ (κ upper bound on sect. Curv. on M with convention that $1/\sqrt{\kappa} = +\infty$ for $\kappa \leq 0$)

Empirical mean (finite sample): almost surely unique!

[Arnaudon & Miclo 2013]

Algorithms to compute the mean

Karcher flow (gradient descent)

$$\bar{x}_{t+1} = \exp_{\bar{x}_t}(\epsilon_t v_t) \text{ with } v_t = E(\overline{y\mathbf{x}}) = \frac{1}{n} \sum_i \log_{\bar{x}_t}(x_i)$$

- Usual algorithm with $\epsilon_t = 1$ can diverge on SPD matrices [Bini & Iannazzo, Linear Algebra Appl., 438:4, 2013]
- Convergence for non-negative curvature (p-means) [Afsari, Tron and Vidal, SICON 2013]

Inductive / incremental weighted means

- $\bar{x}_{k+1} = \exp_{\bar{x}_k} \left(\frac{1}{k} v_k \right)$ with $v_k = \log_{\bar{x}_k}(x_{k+1})$
- On negatively curved spaces [Sturm 2003],
BHV centroid [Billera, Holmes, Vogtmann, 2001]
- On non-positive spaces [G. Cheng, J. Ho, H. Salehian, B. C. Vemuri 2016]

Stochastic algorithm

- [Arnaudon & Miclo, Stoch. Processes and App. 124, 2014]

Distributions for parametric tests

Generalization of the Gaussian density:

- Stochastic heat kernel $p(x,y,t)$ [complex time dependency]
- Wrapped Gaussian [Infinite series difficult to compute]
- Maximal entropy knowing the mean and the covariance

$$N(y) = k \exp(-\beta^t \overrightarrow{\bar{x}\bar{x}} - \frac{1}{2} \overrightarrow{\bar{x}\bar{x}}^t \Gamma \overrightarrow{\bar{x}\bar{x}})$$

$\beta = 0$ for symmetric spaces

$$\Gamma = \Sigma^{(-1)} - \frac{1}{3} \text{Ric} + O(\sigma) + \varepsilon(\sigma / r)$$

$$k = (2\pi)^{-n/2} \cdot \det(\Sigma)^{-1/2} \cdot (1 + O(\sigma^3) + \varepsilon(\sigma / r))$$

Mahalanobis D2 distance / test:

$$\mu_{\mathbf{x}}^2(y) = \overrightarrow{\bar{x}\bar{y}}^t \cdot \Sigma_{\mathbf{xx}}^{(-1)} \cdot \overrightarrow{\bar{x}\bar{y}}$$

- Any distribution:

$$E[\mu_{\mathbf{x}}^2(\mathbf{x})] = n$$

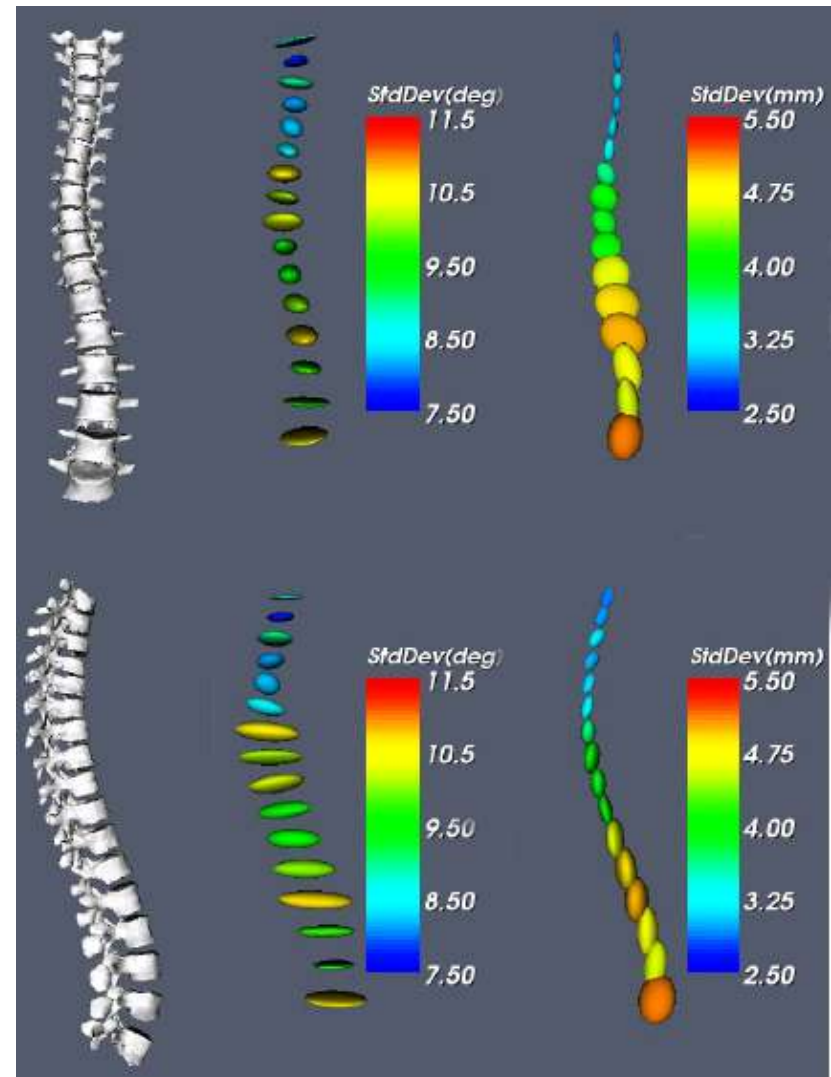
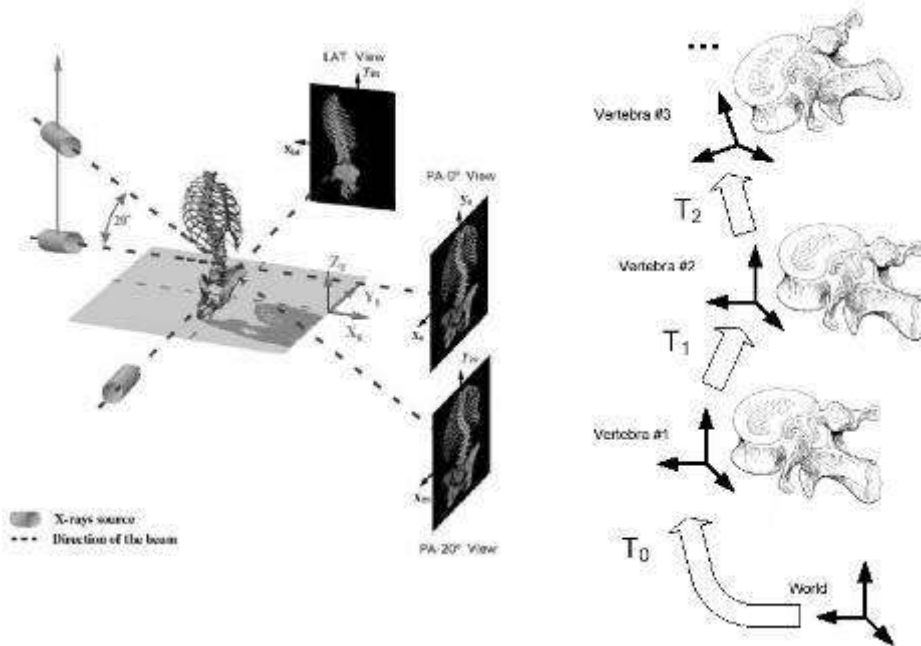
- Gaussian:

$$\mu_{\mathbf{x}}^2(\mathbf{x}) \propto \chi_n^2 + O(\sigma^3) + \varepsilon(\sigma / r)$$

[Pennec, NSIP'99, JMIV 2006]

Statistical Analysis of the Scoliotic Spine

[J. Boisvert et al. ISBI'06, AMDO'06 and IEEE TMI 27(4), 2008]



Database

- 307 Scoliotic patients from the Montreal's Sainte-Justine Hospital.
- 3D Geometry from multi-planar X-rays

Left invariant Mean on $(SO_3 \times R^3)^{16}$

- Main translation variability is axial (growth?)
- Main rot. var. around anterior-posterior axis

Statistical Analysis of the Scoliotic Spine

[J. Boisvert et al. ISBI'06, AMDO'06 and IEEE TMI 27(4), 2008]
AMDO'06 best paper award, Best French-Quebec joint PhD 2009



PCA of the Covariance:

4 first variation modes
have clinical meaning

- Mode 1: King's class I or III
- Mode 2: King's class I, II, III
- Mode 3: King's class IV + V
- Mode 4: King's class V (+II)

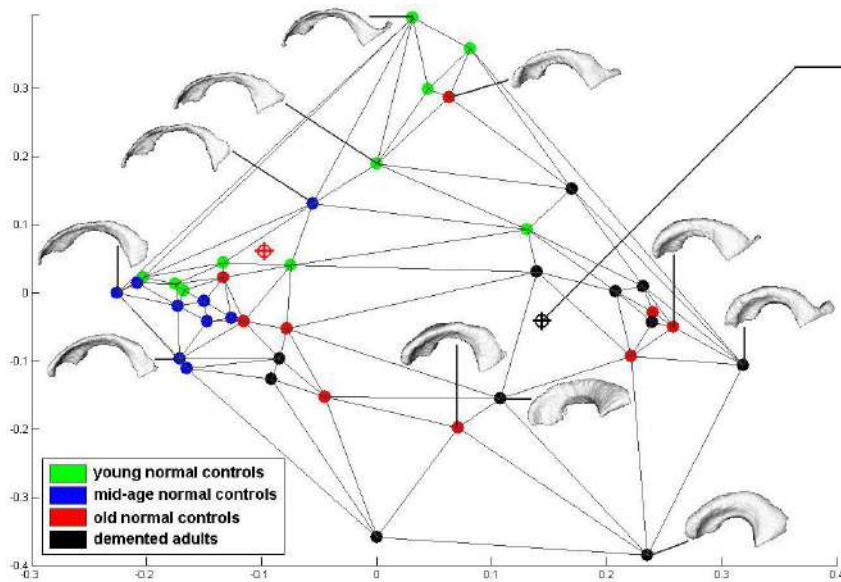
Shape Spaces and Geometric Statistics

Shape spaces: quotient or not quotient?

Geometric statistics

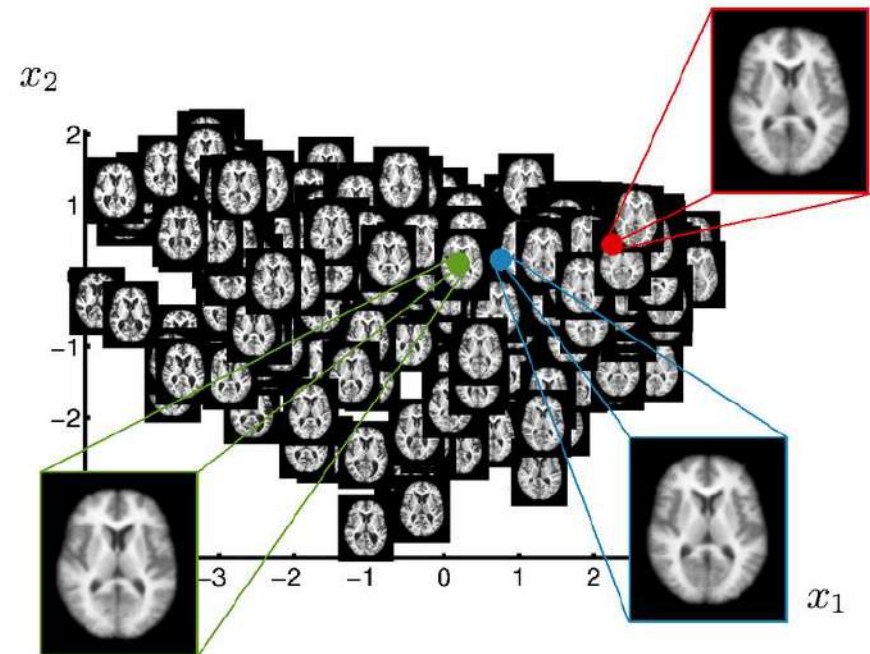
- Simple statistics on Riemannian manifolds
- **Subspaces for PCA in manifolds**
- Some perspectives and open problems

Low dimensional subspace approximation?



Manifold of cerebral ventricles

Etyngier, Keriven, Segonne 2007.



Manifold of brain images

S. Gerber et al, Medical Image analysis, 2009.

- Manifold dimension reduction
- When embedding structure is already manifold (e.g. Riemannian):
Not manifold learning (LLE, Isomap,...) but **submanifold learning**

Tangent PCA

Maximize the squared distance to the mean (explained variance)

- Algorithm
 - Find the Karcher mean \bar{x} minimizing $\sigma^2(x) = \sum_i \text{dist}^2(x, x_i)$
 - Unfold data on tangent space at the mean
 - Diagonalize covariance $\Sigma(x) \propto \sum_i \overrightarrow{\bar{x}x_i} \overrightarrow{\bar{x}x_i}^t$

- Generative model:
 - Gaussian (large variance) in the horizontal subspace
 - Gaussian (small variance) in the vertical space

- Find the subspace of $T_x M$ that best explains the variance

Principal Geodesic / Geodesic Principal Component Analysis

Minimize the squared Riemannian distance to a low dimensional subspace (unexplained variance)

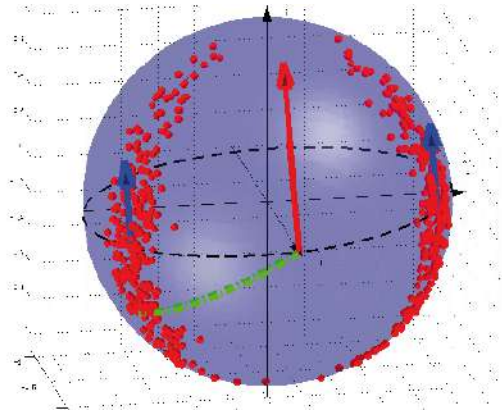
- PGA (Fletcher et al., 2004, Sommer 2014):
space generated by geodesics rays originating from Karcher mean:
$$GS(x, w_1, \dots, w_k) = \{ \exp_x(\sum_i \alpha_i w_i) \text{ for } \alpha \in R^k \}$$
- Geodesic PCA (GPCA, Huckeman et al., 2010):
space generated by principal geodesics that cross at one point
(principal mean, may be different from Karcher mean)
- Generative model:
 - Unknown (uniform ?) distribution within the subspace
 - Gaussian distribution in the vertical space
 - **Beware: GS have to be restricted to be well posed**

All different models in curved spaces (no Pythagore thm)

Problems of tPCA / PGA

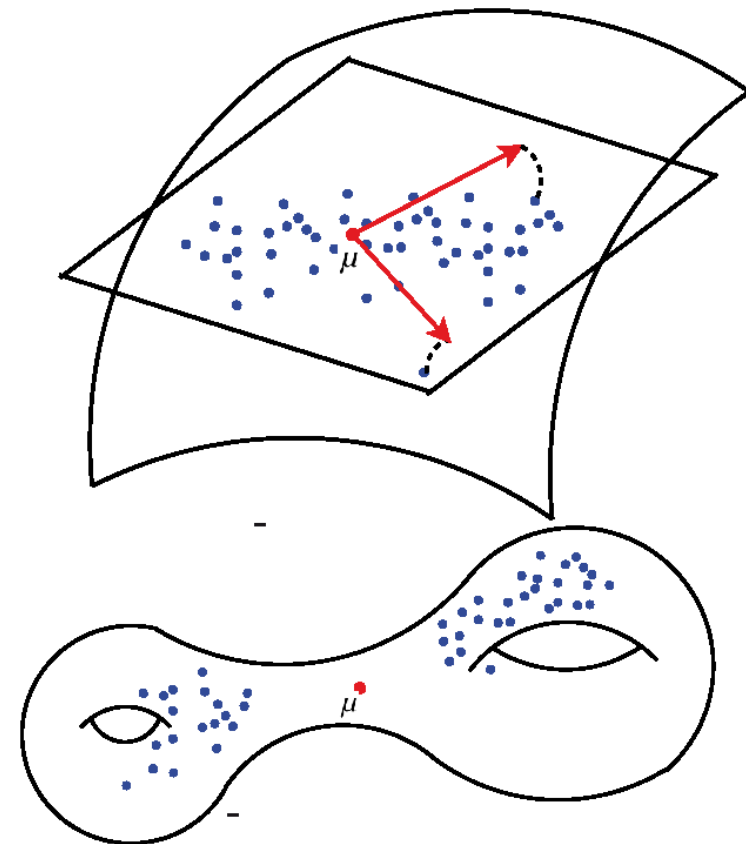
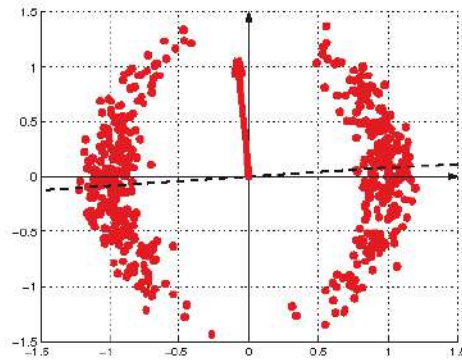
Analysis is done relative to on point

- What if this point is a poor description of the data?
 - Multimodal distributions
 - Uniform distribution on subspaces
 - Large variance w.r.t curvature



Bimodal distribution on S^2

Courtesy of S. Sommer



Courtesy of S. Sommer

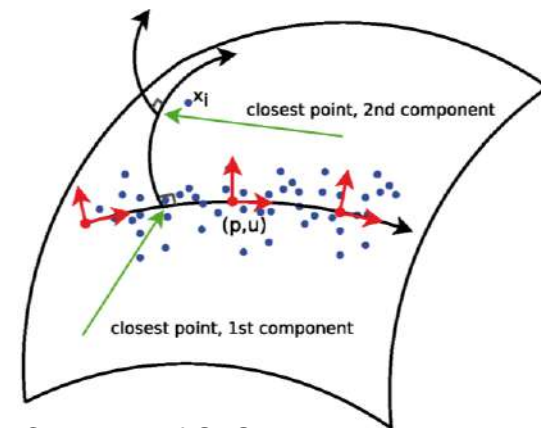
Patching the Problems of tPCA / PGA

Improve the flexibility of the geodesics

- 1D regression with higher order splines [Vialard, Singh, Niethammer]
- Control of dimensionality for n-D Polynomials on manifolds?

Iterated Frame Bundle Development [HCA, Sommer GSI 2013]

- Iterated construction of subspaces
- Parallel transport in frame bundle
- Intrinsic asymmetry between components



Courtesy of S. Sommer

Nested “algebraic” subspaces

- Principal nested spheres [Jung, Dryden, Marron 2012]
- Quotient of Lie group action [Huckemann, Hotz, Munk, 2010]
- No general semi-direct product space structure in general Riemannian manifolds

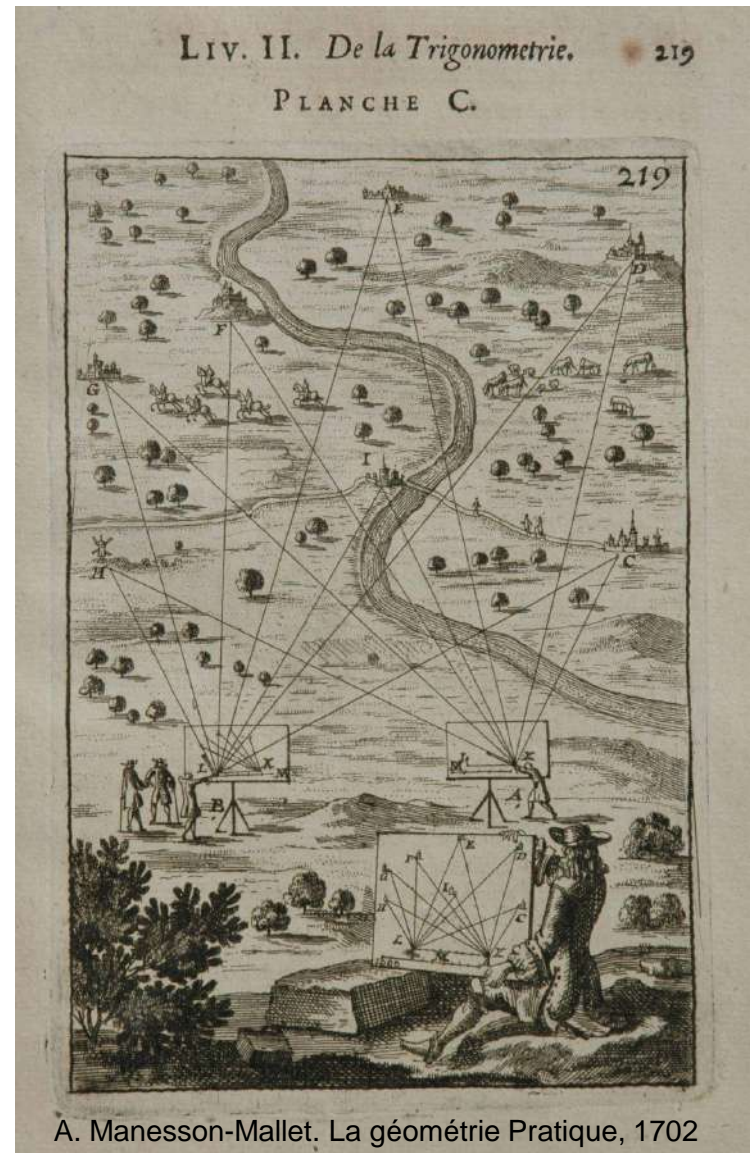
Affine span in Euclidean spaces

Affine span of $(k+1)$ points: weighted barycentric equation

$$\begin{aligned}\text{Aff}(x_0, x_1, \dots, x_k) &= \{x = \sum_i \lambda_i x_i \text{ with } \sum_i \lambda_i = 1\} \\ &= \{x \in R^n \text{ s.t. } \sum_i \lambda_i (x_i - x) = 0, \lambda \in P_k^*\}\end{aligned}$$

Key ideas:

- ~~□ Look at data points from the mean (mean has to be unique)~~
- Look at several reference points from any point of the manifold subspace
- locus of weighted mean



Barycentric subspaces and Affine span in Riemannian manifolds

Fréchet / Karcher barycentric subspaces (KBS / FBS)

- Normalized weighted variance: $\sigma^2(x, \lambda) = \sum \lambda_i \text{dist}^2(x, x_i) / \sum \lambda_i$
- Set of absolute / local minima of the weighted variance
- Works in stratified spaces (may go accross different strata)
 - Non-negative weights: Locus of Fréchet Mean [Weyenberg, Nye]

Exponential barycentric subspace and affine span

- Weighted exponential barycenters: $\mathfrak{M}_1(x, \lambda) = \sum_i \lambda_i \overrightarrow{xx_i} = 0$
- $EBS(x_0, \dots, x_k) = \{x \in M^*(x_0, \dots, x_k) \mid \mathfrak{M}_1(x, \lambda) = 0\}$
- Affine span = closure of EBS in M $Aff(x_0, \dots, x_k) = \overline{EBS(x_0, \dots, x_k)}$

Questions

- KBS/FBS defined by minimization: existence and uniqueness?
- Local structure: local manifold? dimension? stratification?
- Relationship between $KBS \subset FBS$, EBS and affine span?

Analysis of Barycentric Subspaces

Assumptions:

- Restrict to the punctured manifold $M^*(x_0, \dots, x_k) = M \setminus \cup C(x_i)$
- Affinely independent points:
 $\{\overrightarrow{x_i x_j}\}_{0 \leq i \neq j \leq k}$ exist and are linearly indep. for all I

Local well posedness for the barycentric simplex:

- EBS / KBS are well defined in a neighborhood of reference points
- For reference points in a sufficiently small ball and positive weights:
unique Frechet = Karcher = Exp Barycenter in that ball: smooth graph of a k-dim function [proof using Buser & Karcher 81]

SVD characterization of EBS: $\mathfrak{M}_1(x, \lambda) = Z(x)\lambda = 0$

- SVD: $Z(x) = [\overrightarrow{xx_0}, \dots, \overrightarrow{xx_k}] = U(x)S(x)V^t(x)$
 - $EBS(x_0, \dots, x_k) =$ Zero level-set of $l > 0$ singular values of $Z(x)$
 - Stratification on the number of vanishing singular values

Analysis of Barycentric Subspaces

Exp. barycenters are critical points of w-variance on M^*

$$\square \nabla \sigma^2(x, \lambda) = -2\mathfrak{M}_1(x, \lambda) = 0 \quad \mathbf{KBS} \cap M^* \subset \mathbf{EBS}$$

Caractérisation of local minima: Hessian (if non degenerate)

$$H(x, \lambda) = -2 \sum_i \lambda_i D_x \log_x(x_i) = \mathbf{Id} - \frac{1}{3} \mathbf{Ric}(\mathfrak{M}_2(x, \lambda)) + \text{HOT}$$

Regular and positive pts (non-degenerated critical points)

- $\square \mathbf{EBS}^{\text{Reg}}(x_0, \dots, x_k) = \{x \in \text{Aff}(x_0, \dots, x_k), \text{ s. t. } H(x, \lambda^*(x)) \neq \mathbf{0}\}$
- $\square \mathbf{EBS}^+(x_0, \dots, x_k) = \{x \in \text{Aff}(x_0, \dots, x_k), \text{ s. t. } H(x, \lambda^*(x)) \text{ Pos. def.}\}$

Theorem: $\mathbf{KBS} = \mathbf{EBS}^+$ plus potentially some degenerate points of the affine span and some points of the cut locus of the reference points.

X.P. Barycentric Subspace Analysis on Manifolds [arXiv:1607.02833]

KBS / FBS with 3 points on the sphere

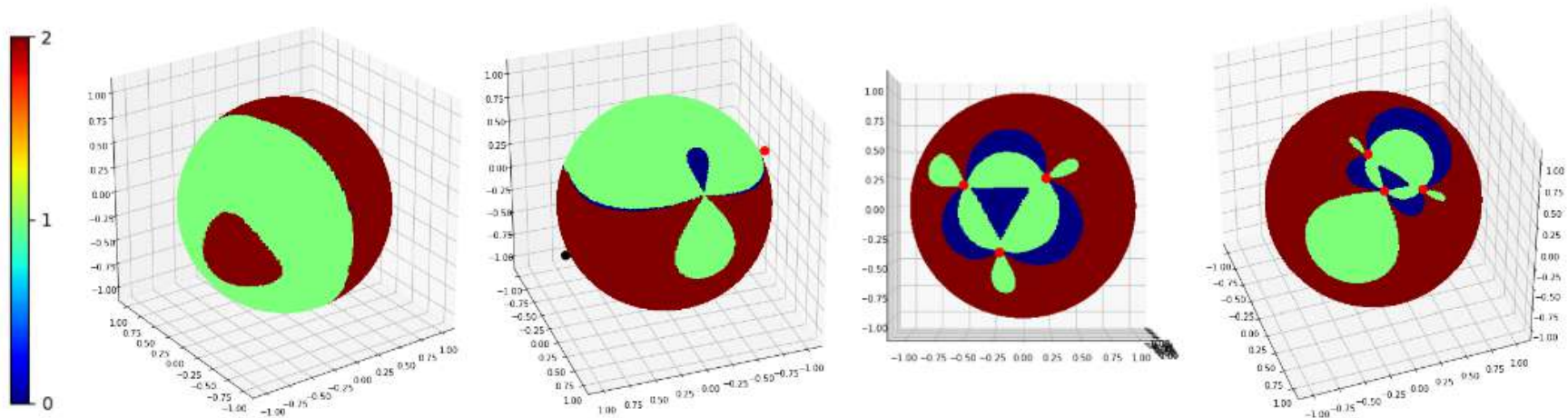
EBS: great subspheres spanned by reference points (mod cut loci)

$$\text{EBS}(x_0, \dots, x_k) = \text{Span}(X) \cap S_n \setminus \text{Cut}(X) \quad \text{Aff}(x_0, \dots, x_k) = \text{Span}(X) \cap S_n$$

Index of the Hessian of weighted variance:

$$H(x, \lambda) = \sum \lambda_i \theta_i \cot(\theta_i) (\text{Id} - xx^t) + \sum (1 - \lambda_i \theta_i \cot(\theta_i)) \overrightarrow{xx_i} \overrightarrow{xx_i}^t$$

- Complex algebraic geometry problem **[Buss & Fillmore, ACM TG 2001]**
- In practice positive & negative eigenvalues: KBS/FBS is a strict and incomplete subset of EBS (**less interesting than affine span**)



KBS / FBS with 3 points on the hyperbolic space

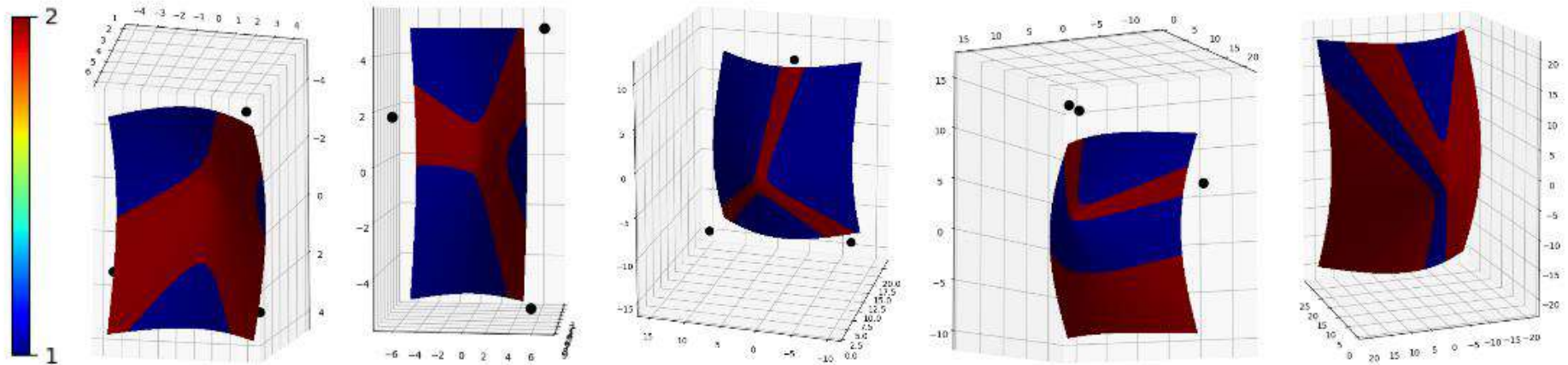
EBS = Affine span: great sub-hyperboloids spanned by reference points

$$\text{EBS}(x_0, \dots, x_k) = \text{Aff}(x_0, \dots, x_k) = \text{Span}(X) \cap H_n$$

Index of the Hessian of weighted variance:

$$H(x, \lambda) = \sum \lambda_i \theta_i \coth(J + J_{XX}^t J^t) + \sum (1 - \lambda_i \coth(\theta_i)) J \overrightarrow{xx_i} \overrightarrow{xx_i}^t J^t$$

- Complex algebraic geometry problem
- Better than for spheres, but still disconnected components



Shape Spaces and Geometric Statistics

Shape spaces: quotient or not quotient?

Geometric statistics

- Simple statistics on Riemannian manifolds
- Subspaces for PCA in manifolds
- **Perspectives, open problems**

Barycentric subspaces

Generalization to α -barycentric subspaces (median, mode)?

- $\sigma^\alpha(x, \lambda) = \frac{1}{\alpha} \sum \lambda_i \text{dist}^\alpha(x, x_i) / \sum \lambda_i$
- Well... critical points of $\sigma^\alpha(x, \lambda)$ are also critical points of $\sigma^2(x, \lambda')$ with $\lambda'_i = \lambda_i \text{dist}^{\alpha-2}(x, x_i)$ (i.e. the affine span)

Limit of affine span for collapsing points

- 1st order: EBS converges to [restricted] Geodesic Subspace
- Conjecture: generalization to non-local higher order (k-n)-jets
 - Principal nested spheres [Jung, Dryden, Marron 2012]
 - Quadratic, cubic splines [Vialard, Singh, Niethammer]
 - Quotient of Lie group action [Huckemann, Hotz, Munk, 2010]

A canonical generalization of affine subspaces in Manifolds?

- Variational formulation? Link with minimal surfaces?

The natural object for PCA: Flags of subspaces in manifolds

Subspace approximations with variable dimension

- Optimal unexplained variance → non nested subspaces
- Nested forward / backward procedures → not optimal
- Optimize first, decide dimension later → Nestedness required
[Principal nested relations: Damon, Marron, JMIV 2014]

Flags of affine spans in manifolds

- $FL(x_0 \prec x_1 \prec \dots \prec x_k)$ sequence of nested subspaces $Aff(x_0, \dots, x_i)$

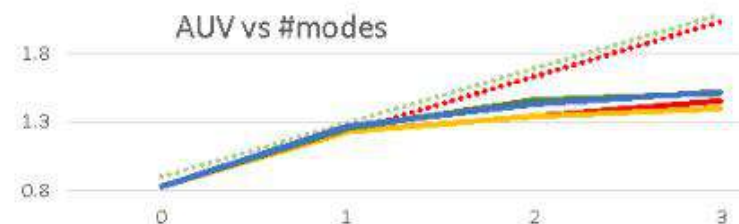
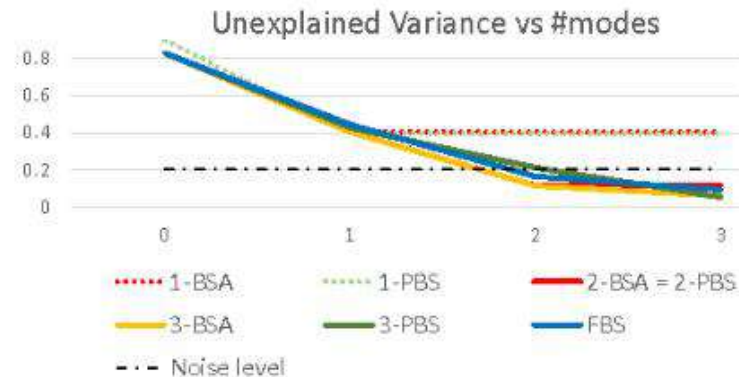
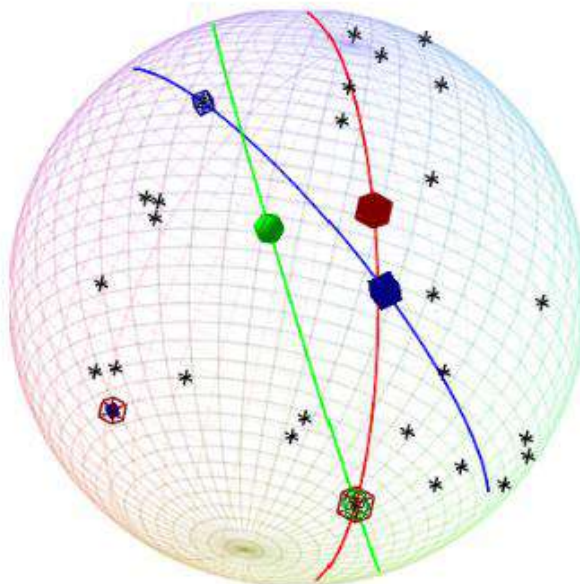
Barycentric subspace analysis (BSA):

- Energy on flags: Accumulated Unexplained Variance
→ produce the right ordered flags of subspaces in Euclidean spaces

X.P. Barycentric Subspace Analysis on Manifolds [arXiv:1607.02833]

Algorithms: Sample-limited inference

- Sample-limited Fréchet mean / template [Lepore et al 2008]
- SL First geodesic mode [Feragen et al. 2013, Zhai et al 2016]
- Higher orders: challenging with PGA... but not with BSA
 - **FBS: Forward Barycentric Subspace**
 - **k-PBS: Pure Barycentric Subspace with backward ordering**
 - **k-BSA: Barycentric Subspace Analysis up to order k**



Geometric statistics: open problems

Riemannian statistics

- Advanced statistics (efficiency, Cramer-Rao, CLT [H. Le, Huckemann])
- Which metric? (least-square ~ isotropic noise)
- Completeness issues (geodesic shooting, projection)
- Boundaries, corners (e.g. pure states in qbits?)

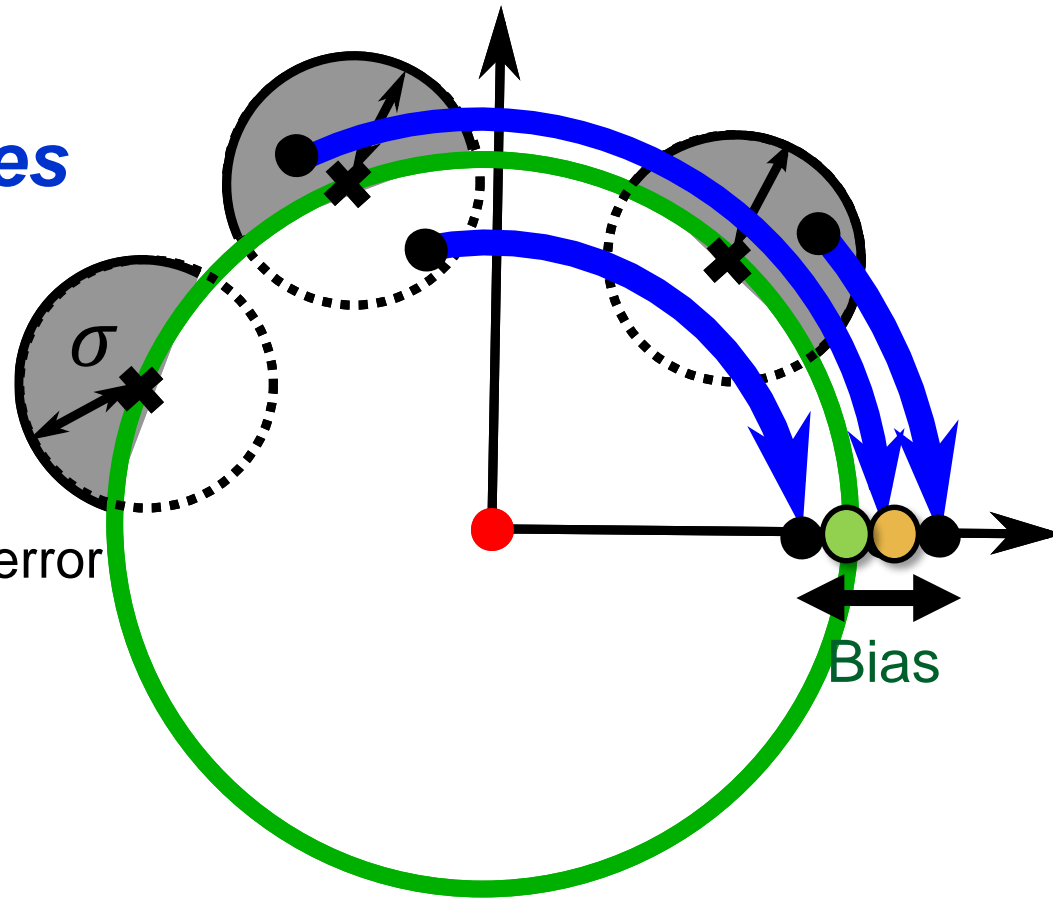
Other geometric structures

- Affine connection spaces?
(bi-invariance on Lie groups with Cartan-Schouten connections)
- Gluing manifolds (e.g. trees)
Log-map well defined [D. Barden, H. Le, 2017]
- Bundles and quotient spaces:
stratification if the isotropy group changes: regular strata not sufficient

Noise in top space = Bias in quotient spaces

σ^2 : variance of
measurement error

The curvature of the
**template shape's
orbit and presence
of noise** creates bias



Theorem [Miolane et al. (2016)]: Bias of estimator \hat{T} of the template T

$$\text{Bias}(\hat{T}, T) = \frac{\sigma^2}{2} \mathbf{H}(T) + \mathcal{O}(\sigma^4)$$

where $\mathbf{H}(T)$: mean curvature vector of **template's orbit**

References on Template bias with in quotient space

- **Manifold of finite dimension, isometric action, asymptotic for $\sigma \rightarrow 0$, correction using bootstrap**

N. Miolane, S. Holmes, X. Pennec. Template shape computation: correcting an asymptotic bias. SIAM Journal of Imaging Science, 10(2):808-844, 2017.

Web applications using Shiny (R): <http://nmiolane.shinyapps.io/shinyPlane/>
[http://nmiolane.shinyapps.io/shinySphere /](http://nmiolane.shinyapps.io/shinySphere/)

- **Hilbert of infinite dimension, proof of bias for $\sigma > 0$, asymptotic for $\sigma \rightarrow \infty$, isometric action:**

L. Devilliers, S. Allasonnière, A. Trouvé and X. Pennec. Template estimation in computational anatomy: Fréchet means in top and quotient spaces are not consistent. SIAM Journal of Imaging Science, 10(3):1139-1169, 2017.

- **Hilbert of infinite dimension, non-isometric action:**

L. Devilliers, S. Allasonnière, A. Trouvé, and X. Pennec. Inconsistency of Template Estimation by Minimizing of the Variance/Pre-Variance in the Quotient Space. Entropy, 19(6):28, June 2017.

- **Quantification of bias? When and how to correct it?**

References on Barycentric Subspace Analysis

- **Barycentric Subspace Analysis on Manifolds [arXiv:1607.02833]**
<https://hal.archives-ouvertes.fr/hal-01343881>
- **Barycentric Subspaces and Affine Spans in Manifolds**
X. Pennec. Geometric Science of Information GSI'2015, Oct 2015, Palaiseau, France. Proceedings of Geometric Science of Information GSI'2015. Springer LNCS 9389, pp.12-21, 2015. http://dx.doi.org/10.1007/978-3-319-25040-3_2 and <https://hal.inria.fr/hal-01164463>
 - Warning: change of denomination since this paper: EBS → affine span
- **Barycentric Subspaces Analysis on Spheres**
X. Pennec. Mathematical Foundations of Computational Anatomy (MFCA'15), Oct 2015, Munich, Germany. pp.71-82, 2015. <https://hal.inria.fr/hal-01203815>
- **Barycentric subspace analysis: a new symmetric group-wise paradigm for cardiac motion tracking**
Marc-Michel Rohé, Maxime Sermesant and Xavier Pennec. Proc of MICCAI 2016, Athens, LNCS 9902, p.300-307, Oct 2016. To appear in Medical Image Analysis.

References for Statistics on Manifolds and Lie Groups

Statistics on Riemannian manifolds

- Xavier Pennec. Intrinsic Statistics on Riemannian Manifolds: Basic Tools for Geometric Measurements. *Journal of Mathematical Imaging and Vision*, 25(1):127-154, July 2006. <http://www.inria.fr/sophia/asclepios/Publications/Xavier.Pennec/Pennec.JMIV06.pdf>

Invariant metric on SPD matrices and of Frechet mean to define manifold-valued image processing algorithms

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Bi-invariant means with Cartan connections on Lie groups

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