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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?

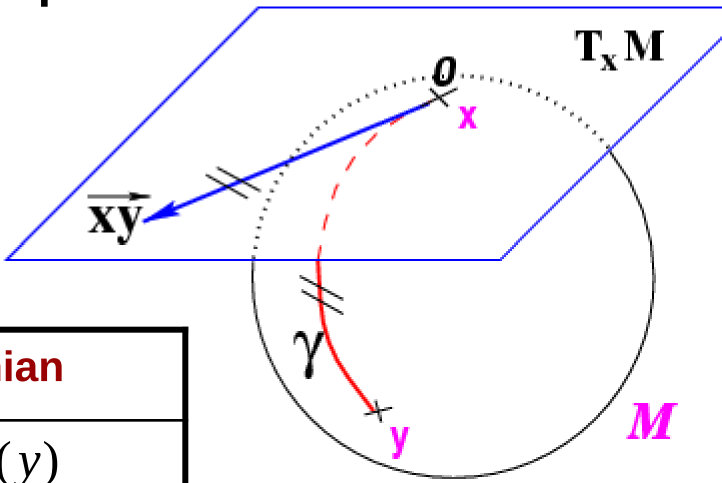
Geometric statistics

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

Computing in Riemannian Manifolds

Exponential map (Normal coordinate system):

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

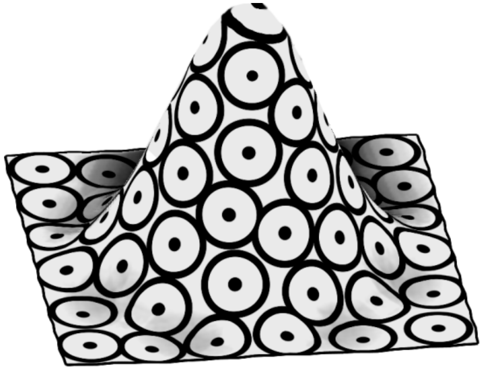


Reformulate algorithms with $\exp_x$ and $\log_x$

Vector -> Bi-point (no more equivalence classes)

Operation	Euclidean space	Riemannian
Subtraction	$\overrightarrow{xy} = y - x$	$\overrightarrow{xy} = \log_x(y)$
Addition	$y = x + \overrightarrow{xy}$	$y = \exp_x(\overrightarrow{xy})$
Distance	$\mathrm{dist}(x,y) = \lVert y - x \rVert$	$\mathrm{dist}(x,y) = \lVert \overrightarrow{xy} \rVert_x$
Gradient descent	$x_{t+\varepsilon} = x_t - \varepsilon \nabla C(x_t)$	$x_{t+\varepsilon} = \exp_{x_t}(-\varepsilon \nabla C(x_t))$

Random variable in a Riemannian Manifold



Intrinsic pdf of x

- For every set H

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

- ~~Lebesgue's measure~~

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

Expectation of an observable in M

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

Statistical tools: Moments

Frechet mean [1944] minimize the variance

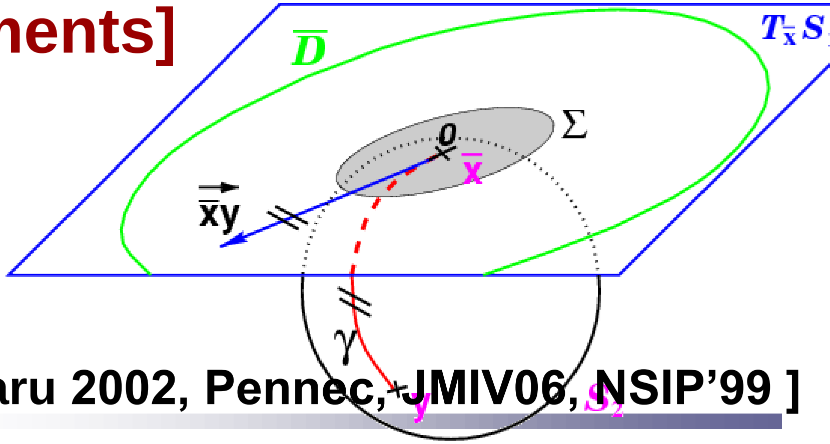
- $\sigma^2(x) = \int_M dist^2(x,z)\, p(z) dM(z)$
- Tensor moments of a random point with density p
  - $\mathfrak{M}_1(x) = \int_M \overrightarrow{xz}\, p(z) dM(z)$ Tangent mean field
  - $\mathfrak{M}_2(x) = \int_M \overrightarrow{xz} \otimes \overrightarrow{xz}\, p(z) dM(z)$ Covariance field

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

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

Covariance [and higher order moments]

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



[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 a regular geodesic ball U(r) with radius $r < r^* = \frac{1}{2}\min(inj(M), \pi/\sqrt{\kappa})$ (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)

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

- 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

$\beta = 0$ for symmetric spaces

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

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

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

Mahalanobis D2 distance / test:

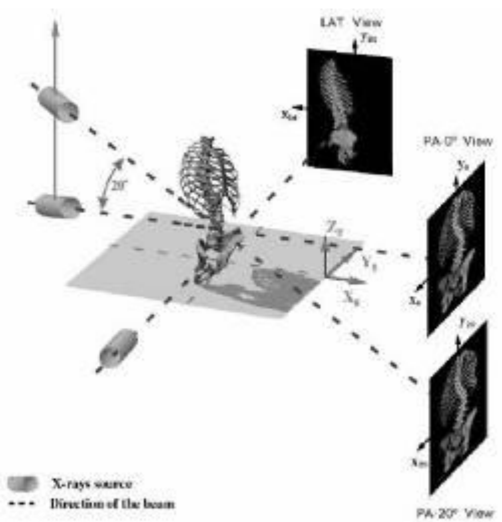
$$\mu_{\mathbf{x}}^2(\mathrm{y}) = \overrightarrow{\bar{\mathrm{x}}\mathrm{y}}^t.\Sigma_{\mathbf{xx}}^{(-1)}.\overrightarrow{\bar{\mathrm{x}}\mathrm{y}}$$

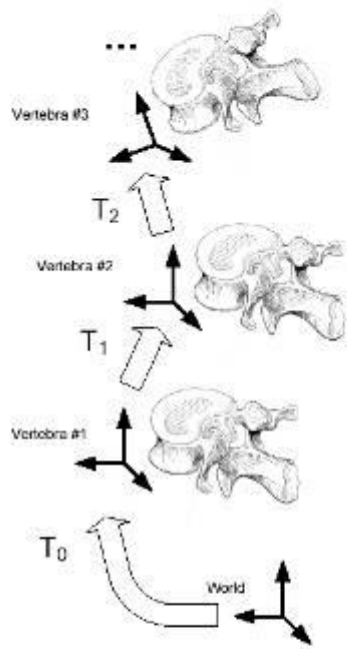
- Any distribution: $\mathrm{E}\left[\mu_{\mathbf{x}}^2(\mathbf{x})\right] = n$
- Gaussian: $\mu_{\mathbf{x}}^2(\mathbf{x}) \propto \chi_n^2 + O(\sigma^3) + \varepsilon(\sigma / r)$

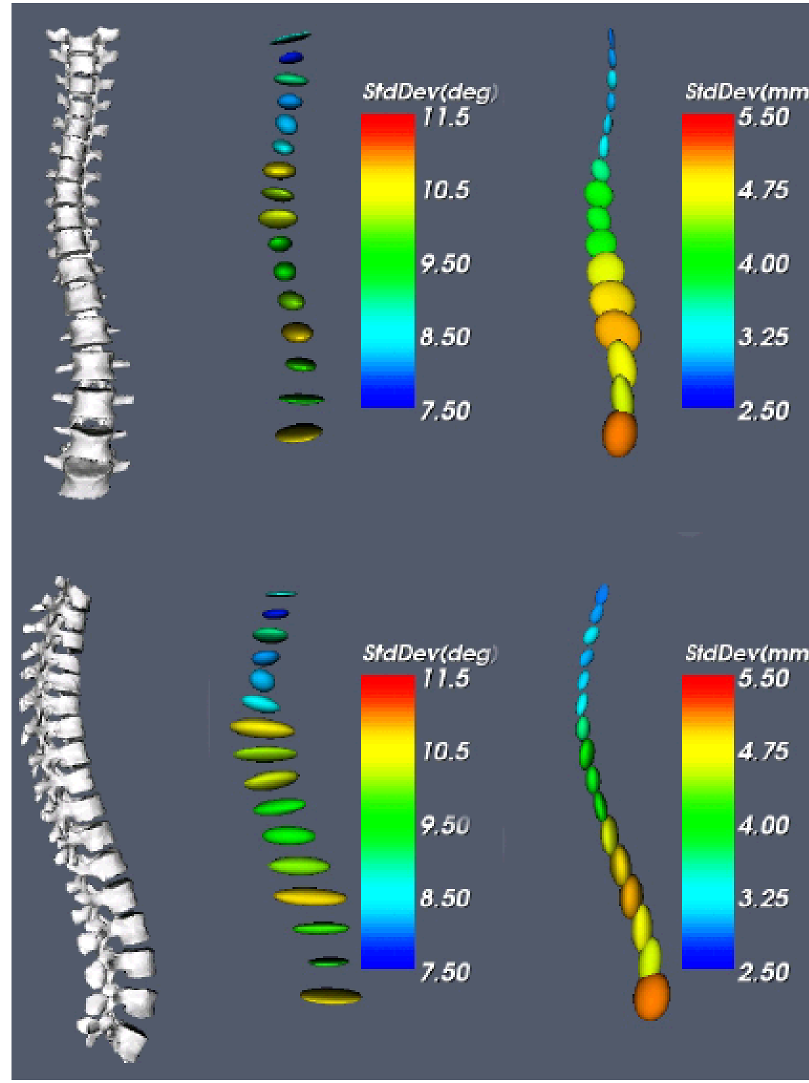
[Pennec, NSIP'99, JMIV 2006]

Statistical Analysis of the Scoliotic Spine

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







Database

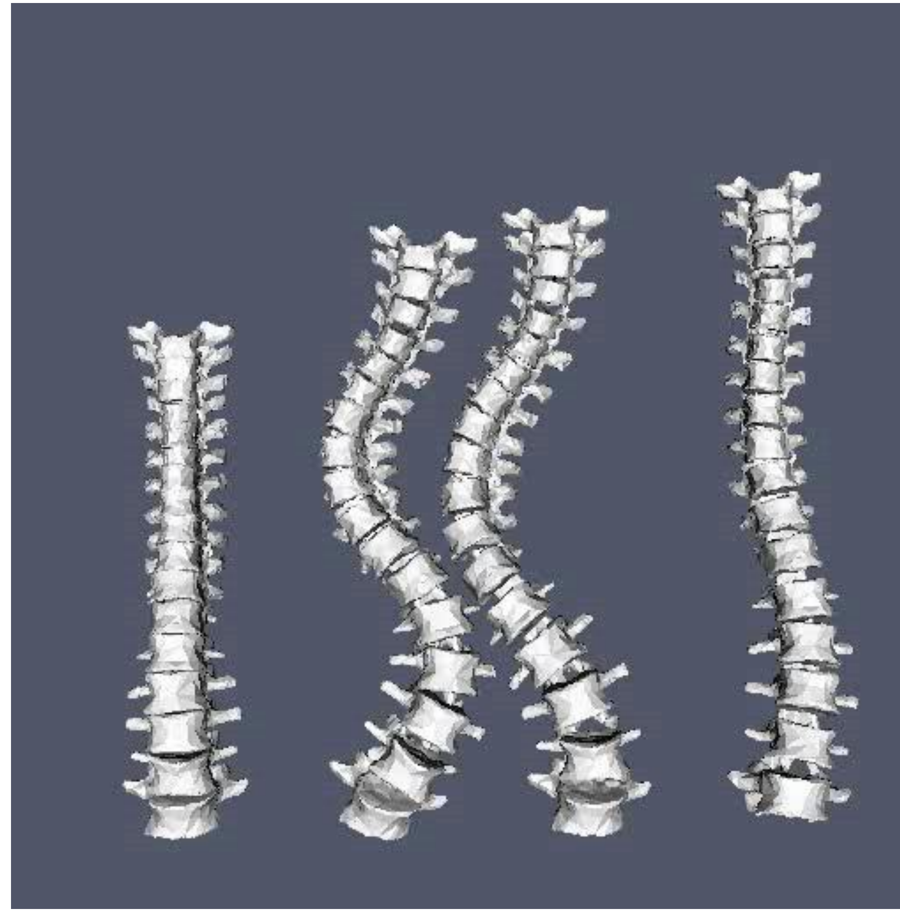
- 307 Scoliotic patients from the Montreal’s Sainte-Justine Hospital.
- 3D Geometry from multi-planar X-rays

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

- 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)

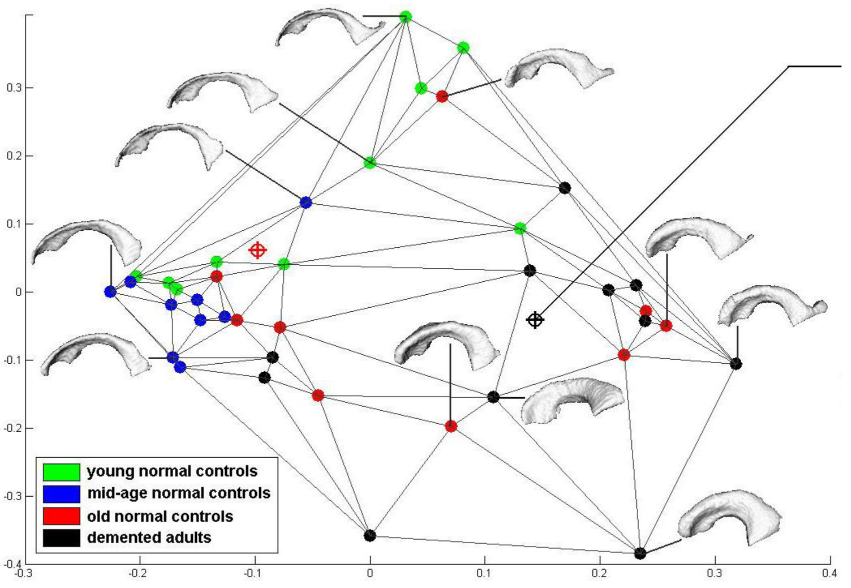
Shape Spaces and Geometric Statistics

Shape spaces: quotient or not quotient?

Geometric statistics

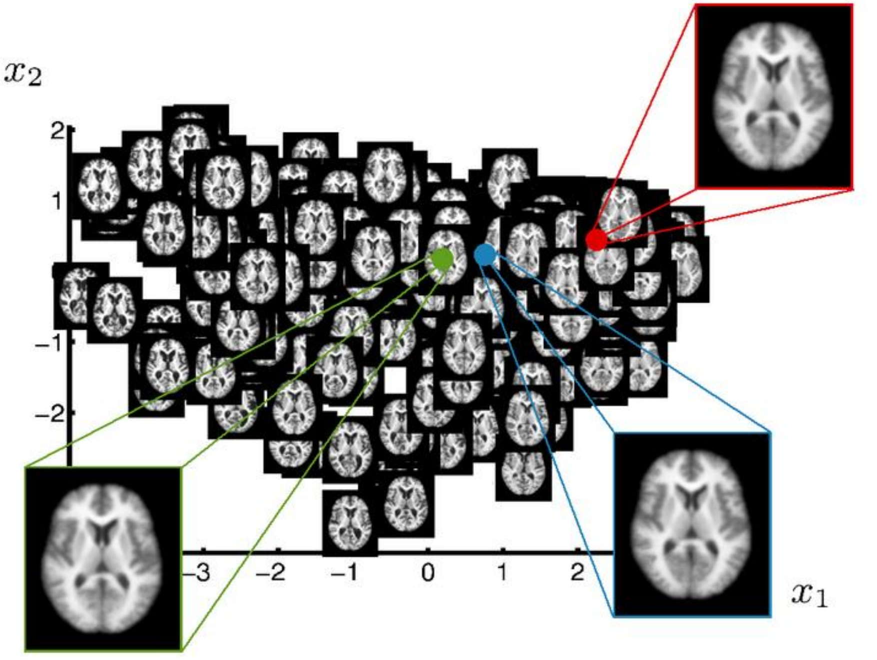
- Simple statistics on Riemannian manifolds
- Subspaces for PCA in manifolds
- Some perspectives and open problems

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 $\sigma^2(x) = \sum_i dist^2(x, x_i)$
  - 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:

  $GS(x, w_1, \dots w_k) = \{\exp_x(\sum_i \alpha_i w_i) \ \ for\ \alpha \in R^k\}$

- 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)

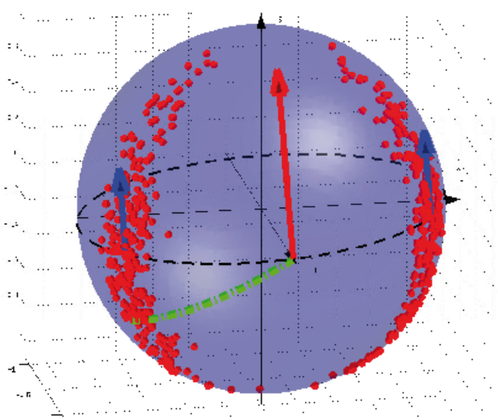
- Generative model:
  - Unknown (uniform ?) distribution within the subspace
  - Gaussian distribution in the vertical space
  - Beware: GS have to be restricted to be well posed

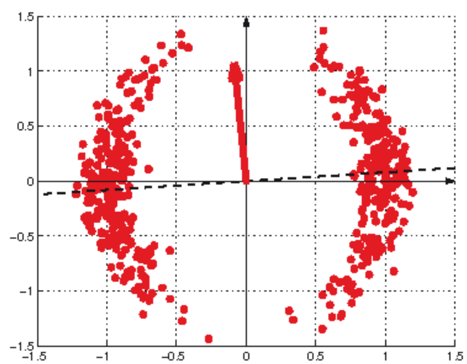
All different models in curved spaces (no Pythagore thm)

Problems of tPCA / PGA

Analysis is done relative to on point

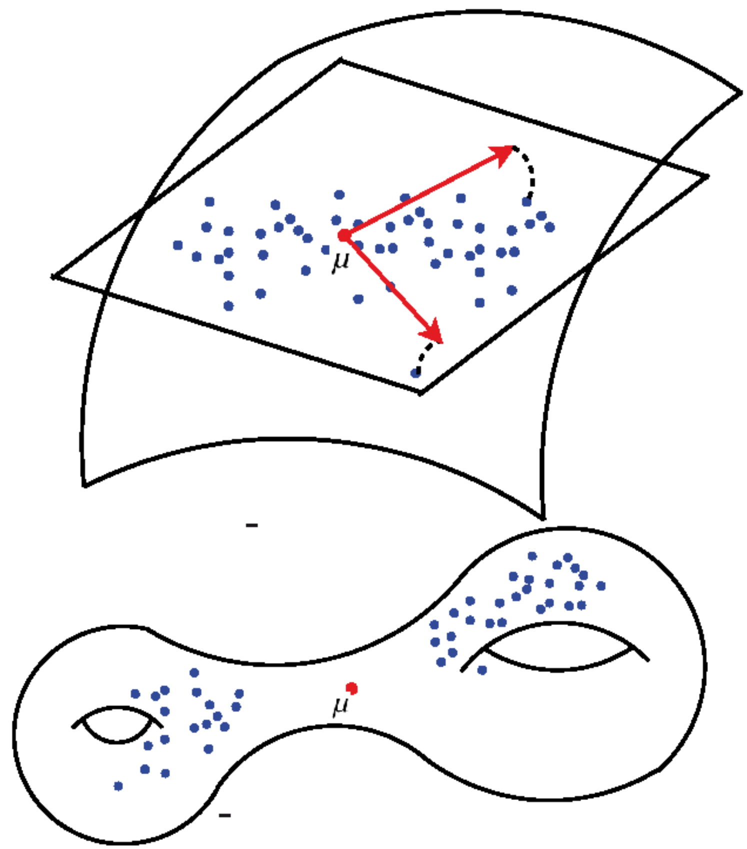
- What if this point is a poor description of the data?
  - Multimodal distributions
  - Uniform distribution on subspaces
  - Large variance w.r.t curvature





Bimodal distribution on S2

Courtesy of S. Sommer



Courtesy of S. Sommer

Patching the Problems of tPCA / PGA

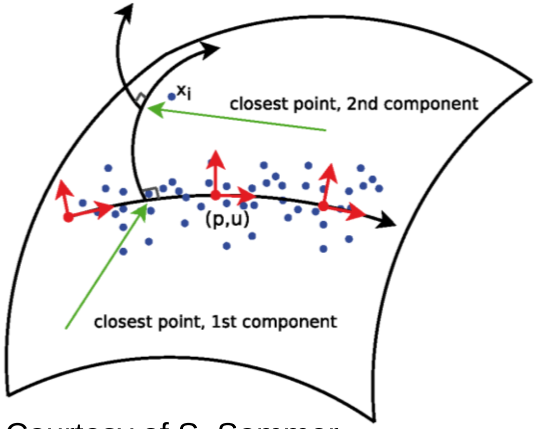
Improve the flexibity of the geodesics

- 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

$$\mathrm{Aff}(\mathrm{x}_0, \mathrm{x}_1, \ldots \mathrm{x}_k) = \{\mathrm{x} = \textstyle\sum_i \lambda_i\, x_i \;\; with \; \sum_i \lambda_i = 1\}$$
$$= \{\mathrm{x} \in R^n \;\; s.t \; \textstyle\sum_i \lambda_i\, (x_i - x) = 0, \lambda \in P_k^*\}$$

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

A. Manesson-Mallet. La géométrie Pratique, 1702

Barycentric subspaces and Affine span in Riemannian manifolds

Fréchet / Karcher barycentric subspaces (KBS / FBS)

- Normalized weighted variance: $\sigma^2(x,\lambda) = \sum \lambda_i dist^2(x, x_i) / \sum \lambda_i$
- 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: $\mathfrak{M}_1(x,\lambda) = \sum_i \lambda_i \overrightarrow{x x_i} = 0$
- $\text{EBS}(x_0, \dots x_k) = \{\, x \in M^*(x_0, \dots x_k) \mid \mathfrak{M}_1(x,\lambda) = 0 \}$
- Affine span = closure of EBS in M $\quad Aff(x_0, \dots x_k) = \overline{EBS(x_0, \dots x_k)}$

Questions

- KBS/FBS defined by minimization: existance and uniqueness?
- Local structure: local manifold? dimension? stratification?
- Relationship between KBS ⊂ FBS, EBS and affine span?

Analysis of Barycentric Subspaces

Assumptions:

- Restrict to the punctured manifold $M^*(x_0, \dots x_k) = M \,/ \cup C(x_i)$
- 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: $\mathfrak{M}_1(\mathrm{x}, \lambda) = Z(x)\lambda = 0$

- 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*

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

Caractérisation of local minima: Hessian (if non degenerate)

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

Regular and positive pts (non-degenerated critical points)

- $\boldsymbol{EBS}^{\boldsymbol{Reg}}(\boldsymbol{x}_0, \ldots \boldsymbol{x}_k) = \{\, \boldsymbol{x} \in \boldsymbol{Aff}(\boldsymbol{x}_0, \ldots \boldsymbol{x}_k), \boldsymbol{s.t.}\ \boldsymbol{H}(\boldsymbol{x}, \boldsymbol{\lambda}^*(\boldsymbol{x})) \neq \mathbf{0}\}$
- $\boldsymbol{EBS}^{+}(\boldsymbol{x}_0, \ldots \boldsymbol{x}_k) = \{\, \boldsymbol{x} \in \boldsymbol{Aff}(\boldsymbol{x}_0, \ldots \boldsymbol{x}_k), \boldsymbol{s.t.}\ \boldsymbol{H}(\boldsymbol{x}, \boldsymbol{\lambda}^*(\boldsymbol{x}))\ \boldsymbol{Pos.def.}\}$

Theorem: $\boldsymbol{KBS} = \boldsymbol{EBS}^{+}$ 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

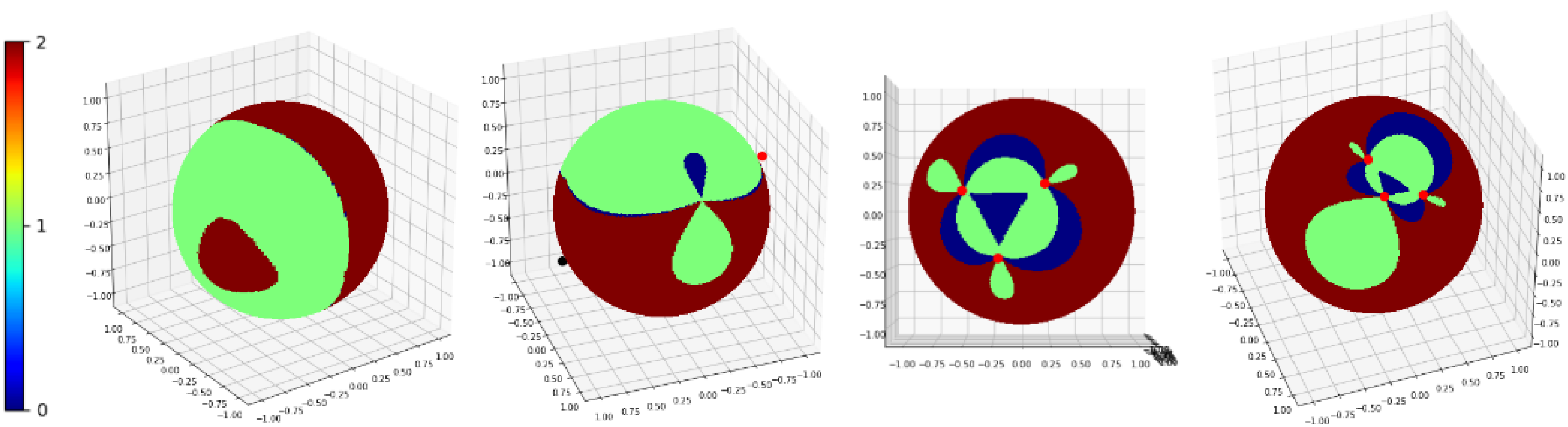
EBS: great subspheres spanned by reference points (mod cut loci)

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

Index of the Hessian of weighted variance:

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

- Complex algebric 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

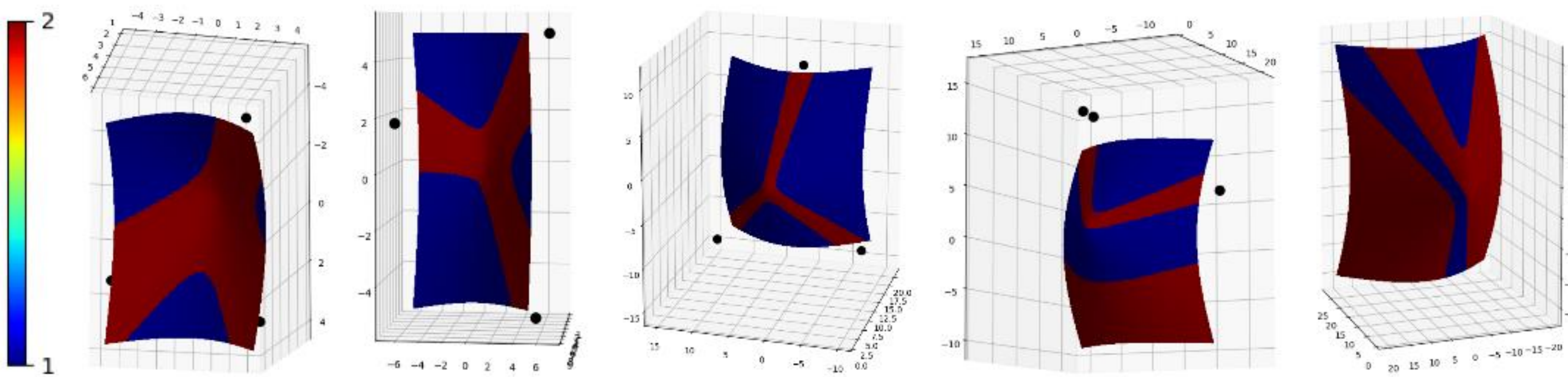
EBS = Affine span: great sub-hyperboloids spanned by reference points

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

Index of the Hessian of weighted variance:

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

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



Shape Spaces and Geometric Statistics

Shape spaces: quotient or not quotient?

Geometric statistics

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- Subspaces for PCA in manifolds
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Barycentric subspaces

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

- $\sigma^{\alpha}(x,\lambda) = \frac{1}{\alpha}\sum\lambda_i dist^{\alpha}(x, x_i)/\sum\lambda_i$
- Well… critical points of $\sigma^{\alpha}(x,\lambda)$ are also critical points of $\sigma^{2}(x,\lambda')$ with $\lambda'_i = \lambda_i\ dist^{\alpha-2}(x, x_i)$ (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

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

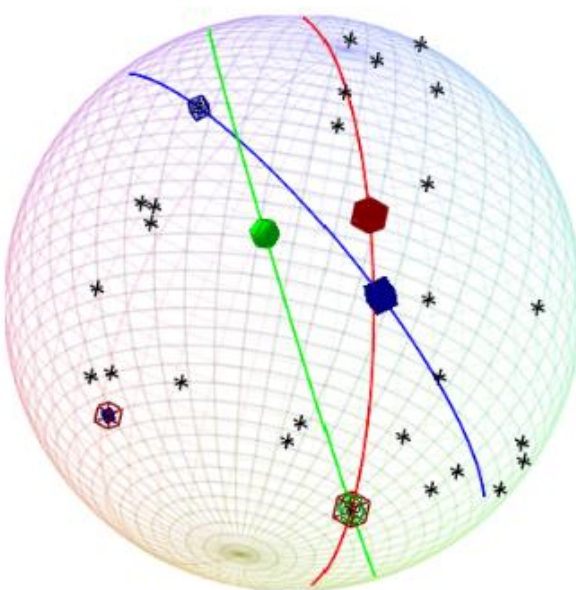
Barycentric subspace analysis (BSA):

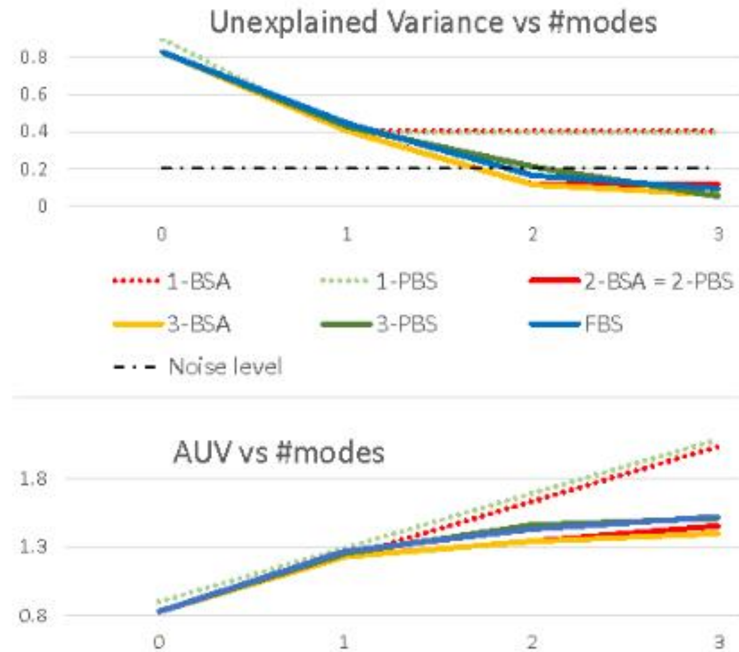
- Energy on flags: Accumulated Unexplained Variance
  → produce the right ordered flags of subspaces in Euclidean spaces

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

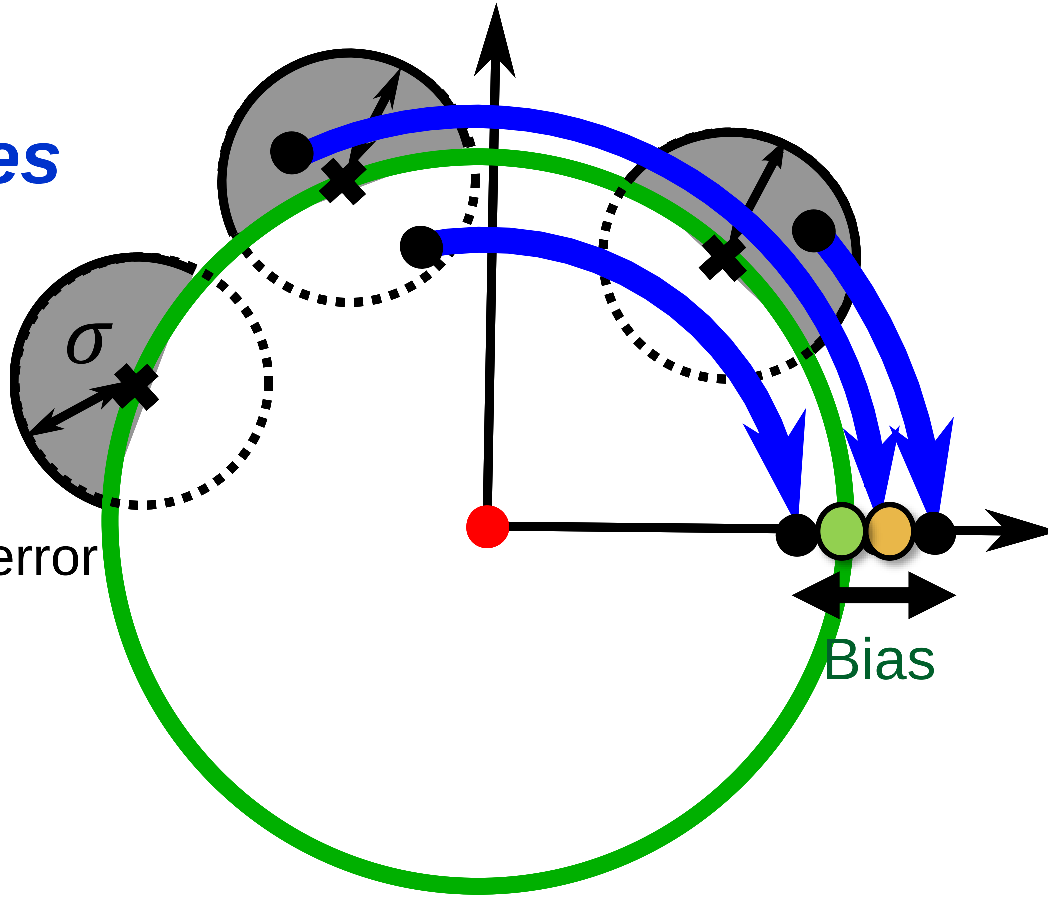
Riemannian statistics

- 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

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

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 $\sigma \to 0$, 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 /

- **Hilbert of infinite dimension, proof of bias for $\sigma > 0$, asymptotic for $\sigma \to \infty$, 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. Allassonnière, 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**
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