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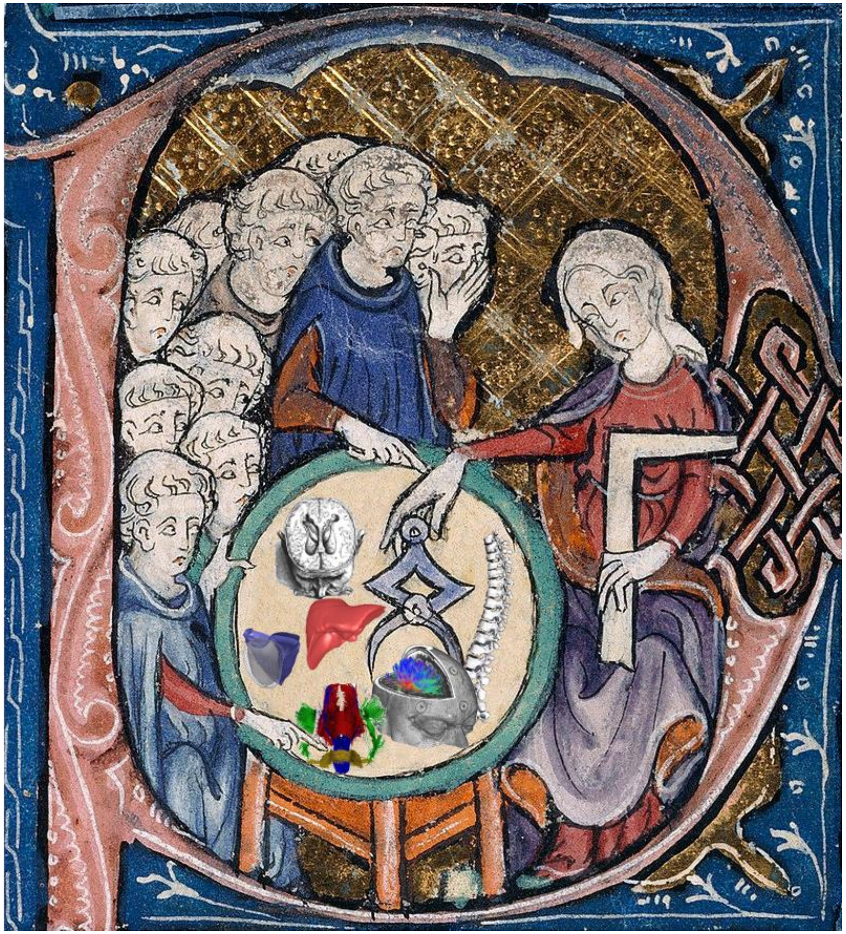
Geometric Statistics

Geometric Statistics for Computational Anatomy

Beyond the Mean Value
Beyond the Riemannian Metric



Freely adapted from "Women teaching geometry", in Adelard of Bath translation of Euclid's elements, 1310.

W. on Geometric Processing
IPAM, April 2, 2019.

Epione e-patient / e-medicine

Inria

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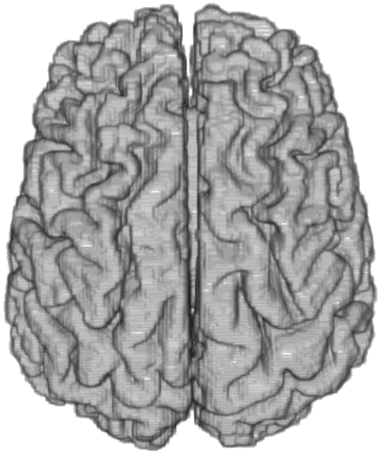
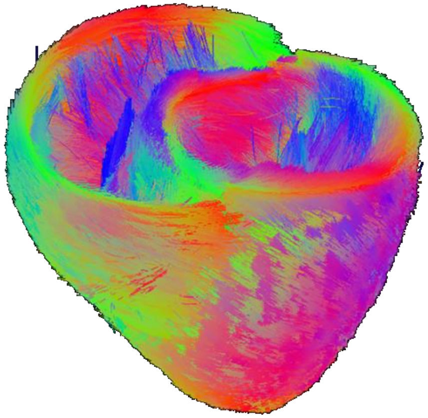
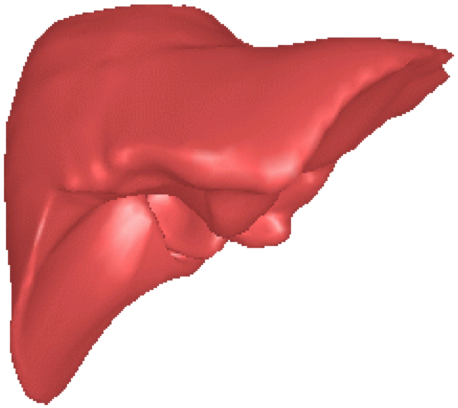
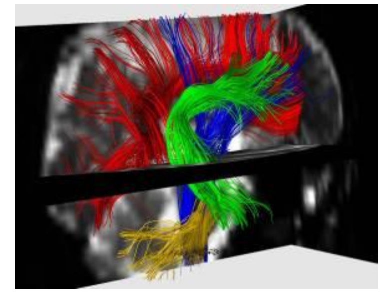
Computational Anatomy


Design mathematical methods and algorithms to model and analyze the anatomy

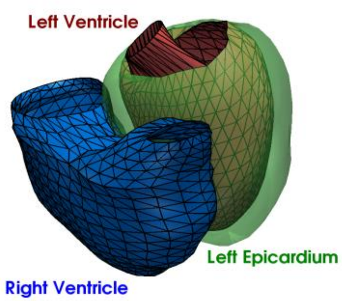
- Statistics of organ shapes across subjects in species, populations, diseases…
  - Mean shape, subspace of normal vs pathologic shapes
  - Shape variability (Covariance)
- Model organ development across time (heart-beat, growth, ageing, ages…)
  - Predictive (vs descriptive) models of evolution
  - Correlation with clinical variables

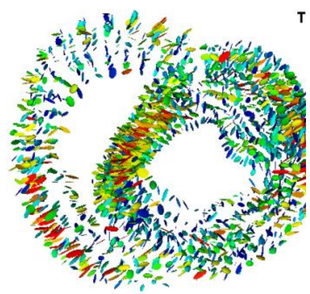
Geometric features in Computational Anatomy

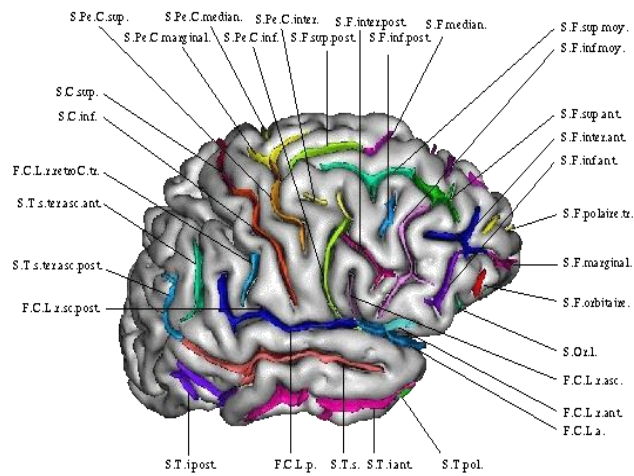


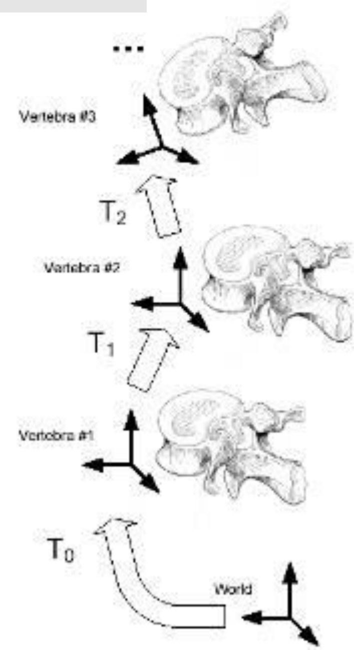
Noisy geometric features

- SPD (covariance) matrices
- Curves, fiber tracts
- Surfaces









- Transformations
  - Rigid, affine, locally affine, diffeomorphisms

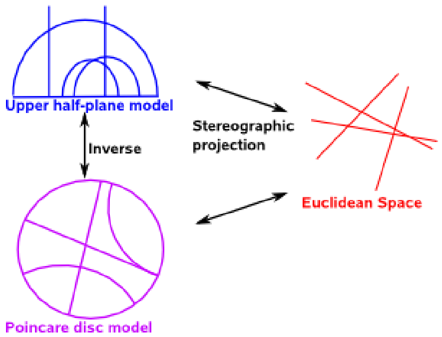
Goal: statistical modeling at the population level

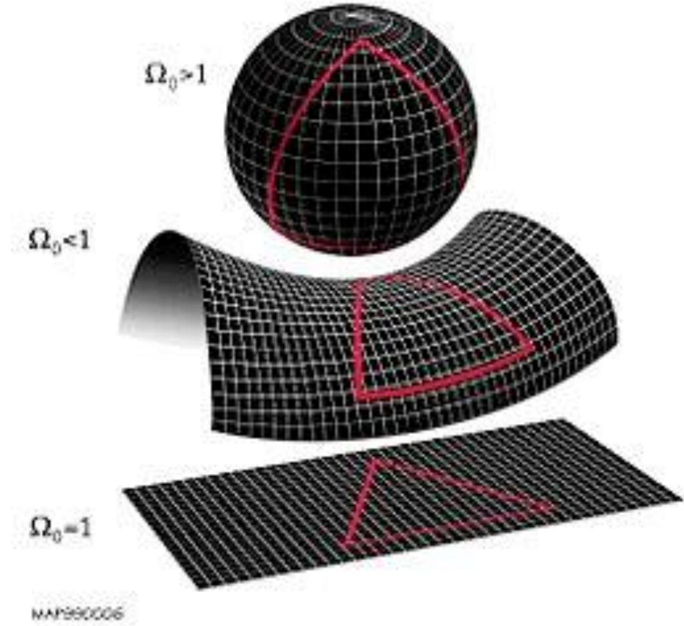
- **Simple statistics on non-Euclidean manifolds (mean, PCA…)**

Hierarchy of Non-linear spaces

Constant curvatures spaces

- Sphere,
- Euclidean,
- Hyperbolic





Lie groups and symmetric spaces

- Riemannian case: compact/non-compact (positive/negative curvature)
- Non-Riemannian cases: change isometry to **affine** transformation

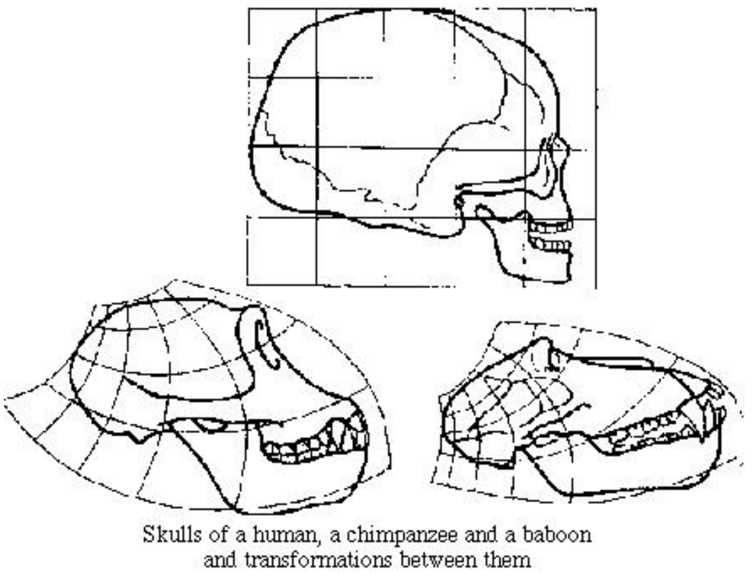
Homogeneous spaces

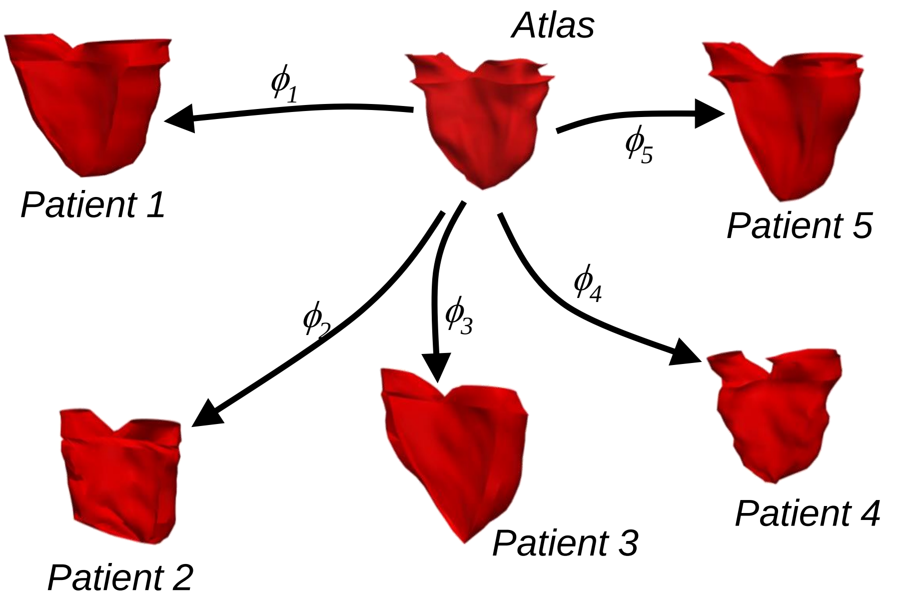
- All points are comparable through a group action

Riemannian or affine spaces

Quotient and stratified spaces

Morphometry through Deformations

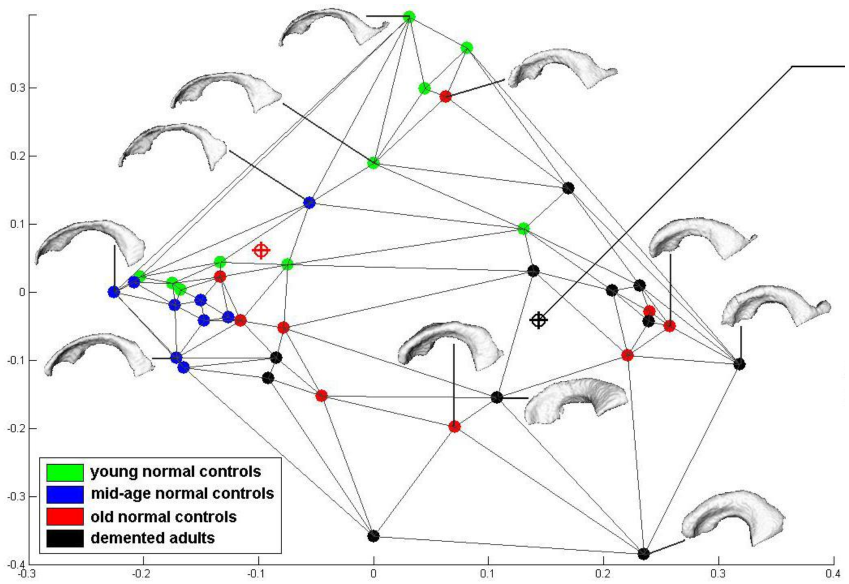




Measure of deformation [D'Arcy Thompson 1917, Grenander & Miller]

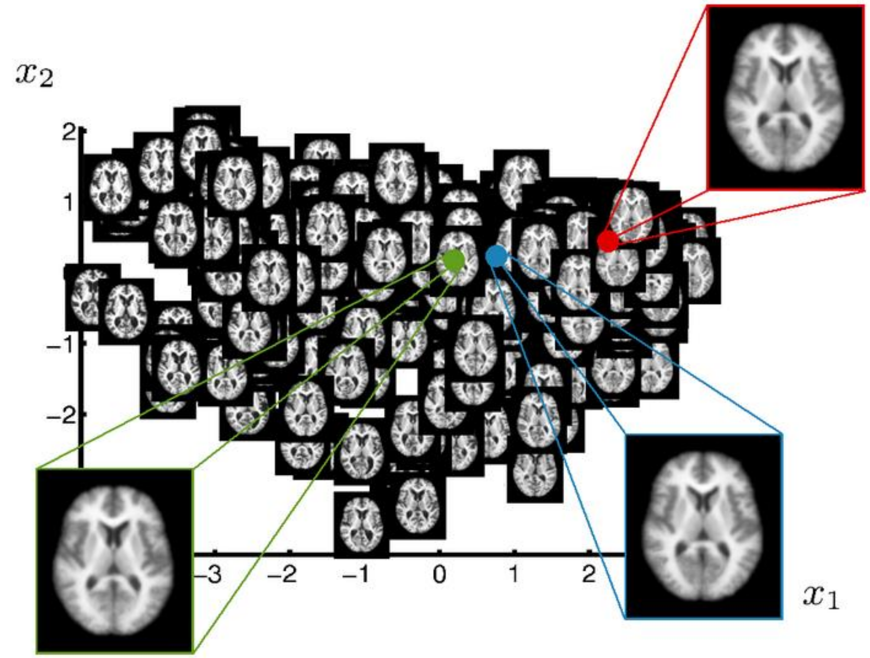
- Reference template = Mean (atlas)
- Shape variability encoded by the "random" template deformations
- Consistent structures for statistics on groups of transformations?
  - No bi-invariant Riemannian metric, but an **invariant symmetric affine connection**

Low dimensional subspace approximation?



Manifold of cerebral ventricles

Etyngier, Keriven, Segonne 2007.



Manifold of brain images

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

- Beyond the 0-dim mean → higher dimensional subspaces
- When embedding structure is already manifold (e.g. Riemannian): Not manifold learning (LLE, Isomap,…) but **submanifold learning**
- **Natural subspaces for extending PCA to manifolds?**

Outline

Statistics beyond the mean

- Basics statistics on Riemannian manifolds
- Barycentric Subspace Analysis: an extension of PCA

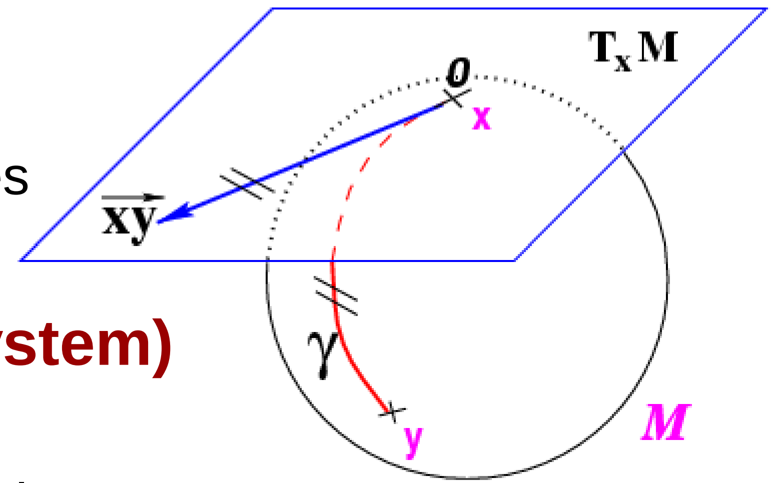
Beyond the Riemannian metric: an affine setting

Conclusions

Bases of Algorithms in Riemannian Manifolds

Riemannian metric:

- Dot product on tangent space
- Geodesics are length minimizing curves



Exponential map (normal coord. System)

- Folding (Exp_x) = geodesic shooting
- Unfolding (Log_x) = boundary value problem
- Geodesic completeness: covers M \ Cut(x)

Operator	Euclidean space	Riemannian manifold
Subtraction	$\overrightarrow{xy} = y - x$	$\overrightarrow{xy} = Log_x(y)$
Addition	$y = x + \overrightarrow{xy}$	$y = Exp_x(\overrightarrow{xy})$
Distance	$\text{dist}(x, y) = \|y - x\|$	$\text{dist}(x, y) = \|\overrightarrow{xy}\|_x$
Gradient descent	$x_{t+\varepsilon} = x_t - \varepsilon \nabla C(x_t)$	$x_{t+\varepsilon} = Exp_{x_t}(-\varepsilon \nabla C(x_t))$

Several definitions of the mean

Tensor moments of a random point on M

- $\mathfrak{M}_1(x) = \int_M \overrightarrow{xz}\, dP(z)$ — Tangent mean: (0,1) tensor field
- $\mathfrak{M}_2(x) = \int_M \overrightarrow{xz} \otimes \overrightarrow{xz}\, dP(z)$ — Covariance: (0,2) tensor field
- $\mathfrak{M}_k(x) = \int_M \overrightarrow{xz} \otimes \overrightarrow{xz} \otimes \cdots \otimes \overrightarrow{xz}\, dP(z)$ — k-contravariant tensor field
- $\sigma^2(x) = Tr_g\big(\mathfrak{M}_2(x)\big) = \int_M dist^2(x,z)\, dP(z)$ — **Variance function**

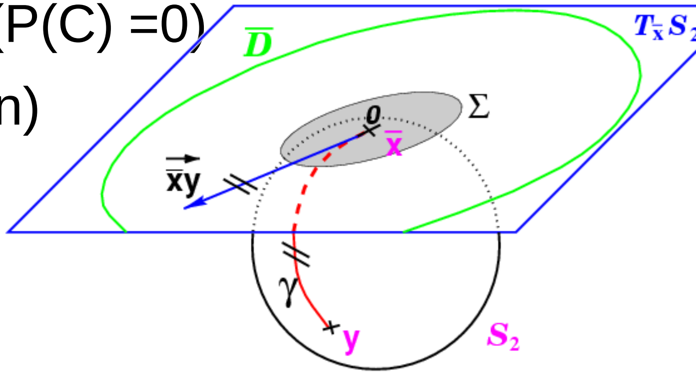
Mean value = optimum of the variance

- **Frechet mean** [1944] = global minima
- **Karcher mean** [1977] = local minima
- **Exponential barycenters** = critical points (P(C) =0)

  $\mathfrak{M}_1(\bar{x}) = \int_M \overrightarrow{\bar{x}z}\, dP(z) = 0$ (implicit definition)

Covariance at the mean

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



Tangent PCA (tPCA)

Maximize the squared distance to the mean (explained variance)

- Algorithm
  - Unfold data on tangent space at the mean
  - Diagonalize covariance at the mean $\Sigma(x) \propto \sum_i \overrightarrow{\bar{x}x_i}\,\overrightarrow{\bar{x}x_i}^t$

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

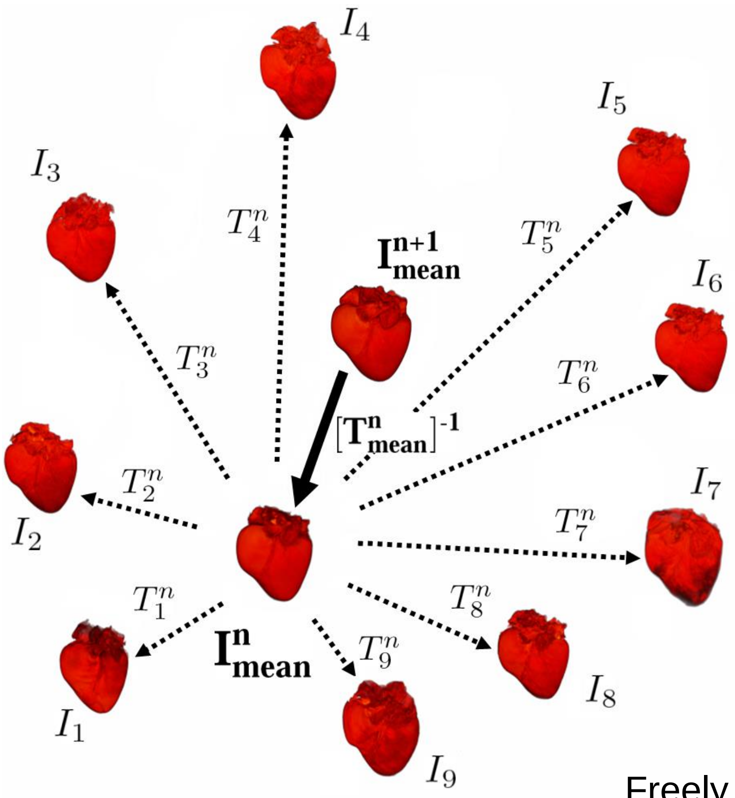
- Find the subspace of T_xM that best explains the variance

A Statistical Atlas of the Cardiac Fiber Structure

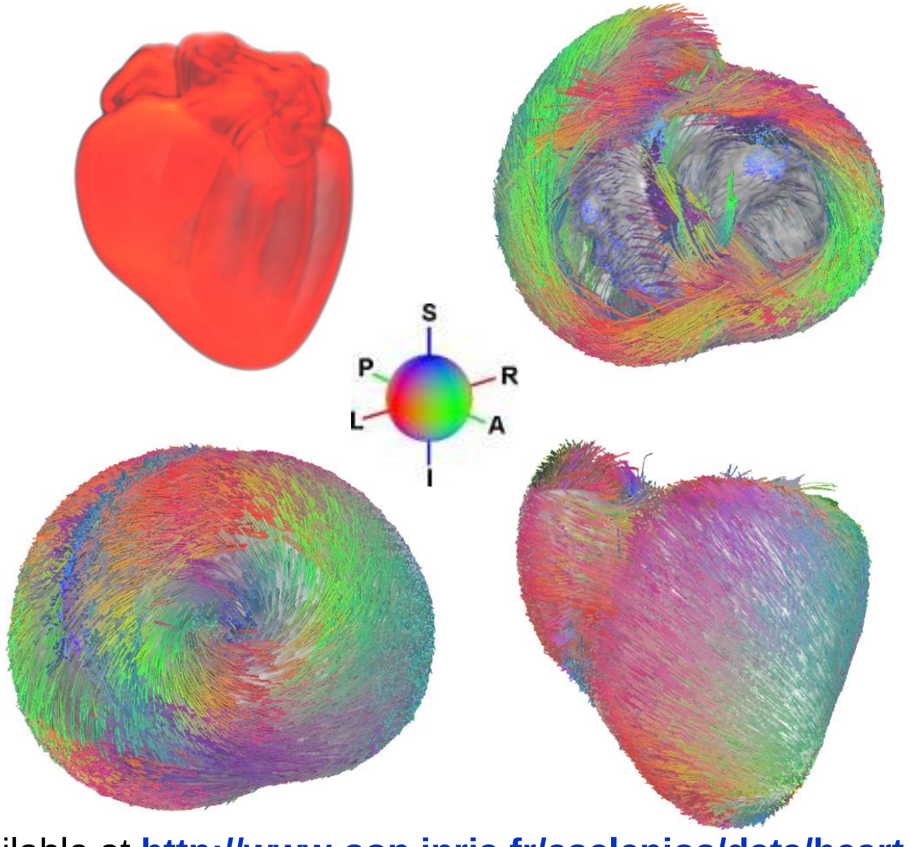
[J.M. Peyrat, et al., MICCAI'06, TMI 26(11), 2007]

Manifold data on a manifold

- Anatomical MRI and DTI
- Diffusion tensor on a 3D shape

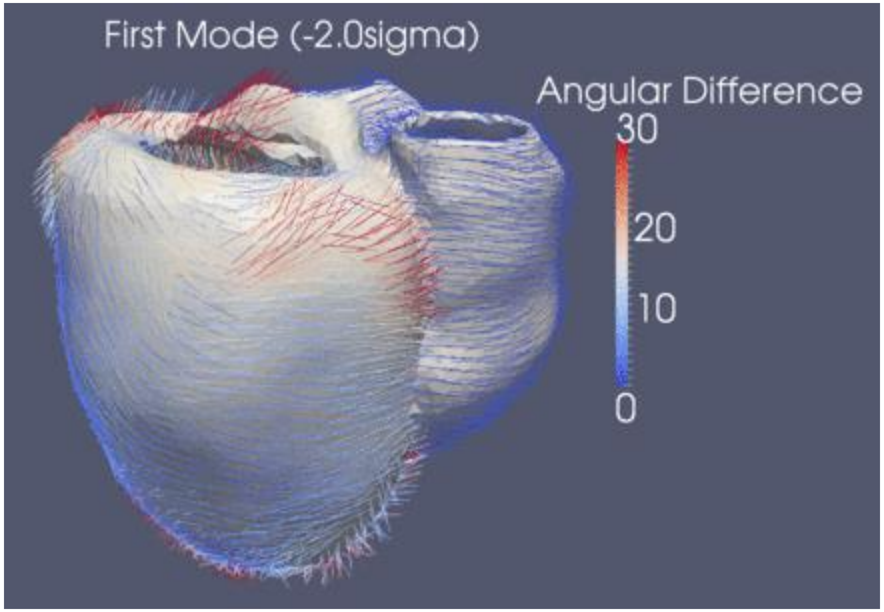


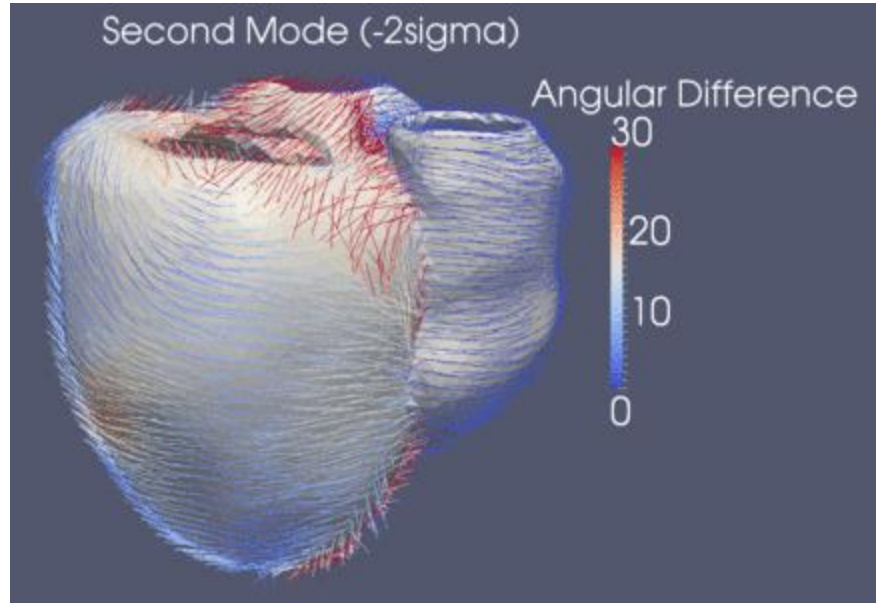
- *Average cardiac structure*
- Variability of fibers, sheets



Freely available at **http://www-sop.inria.fr/asclepios/data/heart**

A Statistical Atlas of the Cardiac Fiber Structure

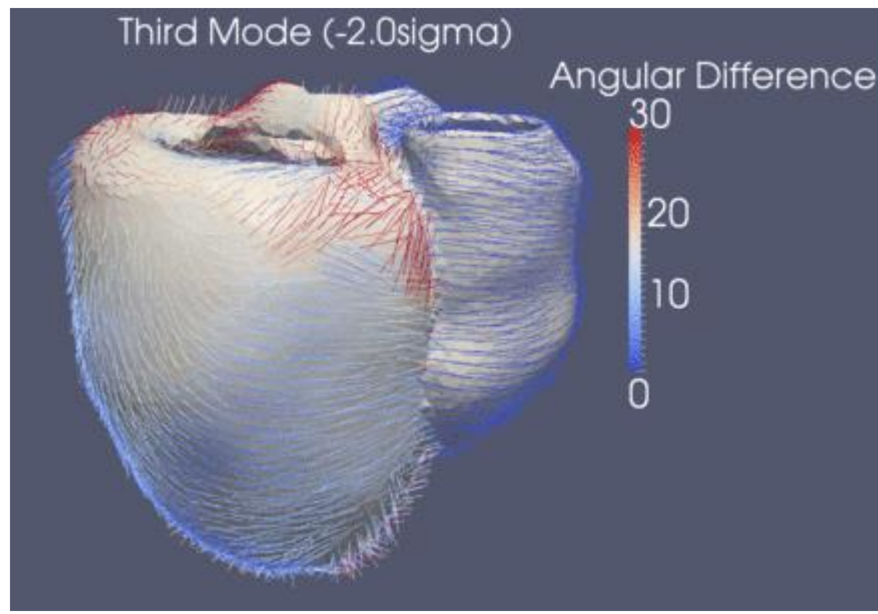




10 human ex vivo hearts (CREATIS-LRMN, France)

- Classified as healthy (controlling weight, septal thickness, pathology examination)
- Acquired on 1.5T MR Avento Siemens
  - bipolar echo planar imaging, 4 repetitions, 12 gradients
- Volume size: 128×128×52, 2 mm resolution

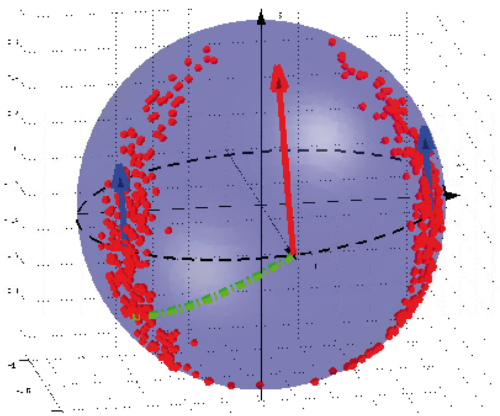
[R. Mollero, M.M Rohé, et al, FIMH 2015]



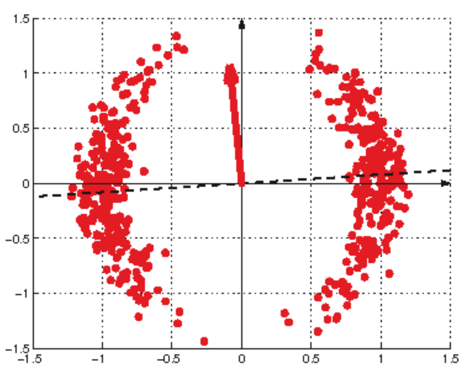
Problems of tPCA

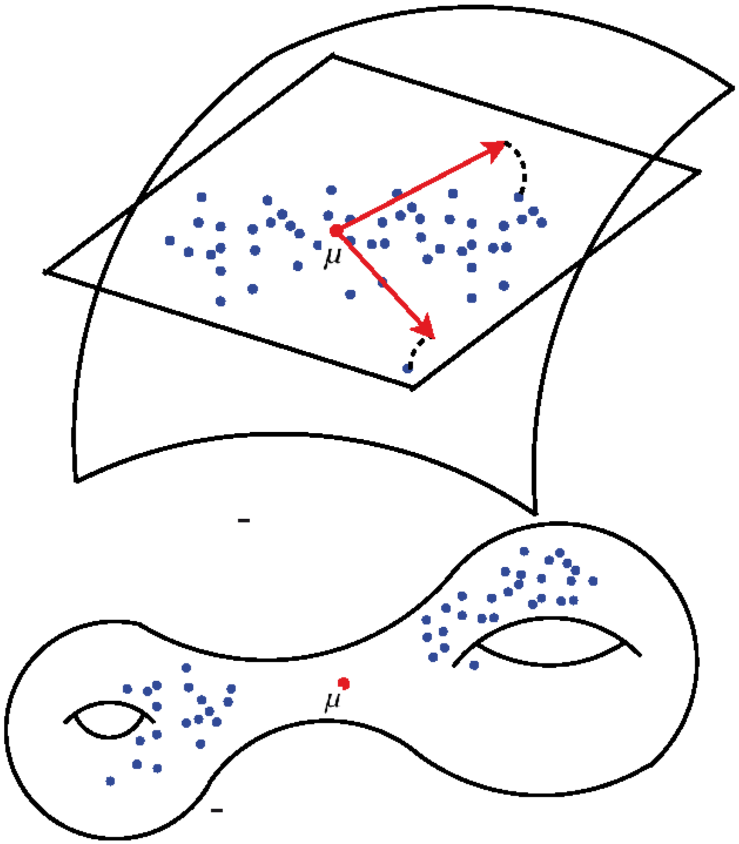
Analysis is done relative to the mean

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



Bimodal distribution on S2





Images courtesy of S. Sommer

Principal Geodesic / Geodesic Principal Component Analysis

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

- **Geodesic Subspace**: $GS(x, w_1, \dots w_k) = \{\exp_x(\sum_i \alpha_i w_i) \;\; for\; \alpha \in R^k\}$
  - Parametric subspace spanned by geodesic rays from point x
  - Beware: GS have to be restricted to be well posed [XP, AoS 2018]
    - PGA (Fletcher et al., 2004, Sommer 2014)
    - Geodesic PCA (GPCA, Huckeman et al., 2010)

- Generative model:
  - Unknown (uniform ?) distribution within the subspace
  - Gaussian distribution in the vertical space

Asymmetry w.r.t. the base point in $GS(x, w_1, \dots w_k)$

- Totally geodesic at x only

Outline

Statistics beyond the mean

- Basics statistics on Riemannian manifolds
- Barycentric Subspace Analysis
  - Natural subspaces in manifolds
  - Rephrasing PCA with flags of subspaces

Beyond the Riemannian metric: an affine setting

Conclusions

Affine span in Euclidean spaces

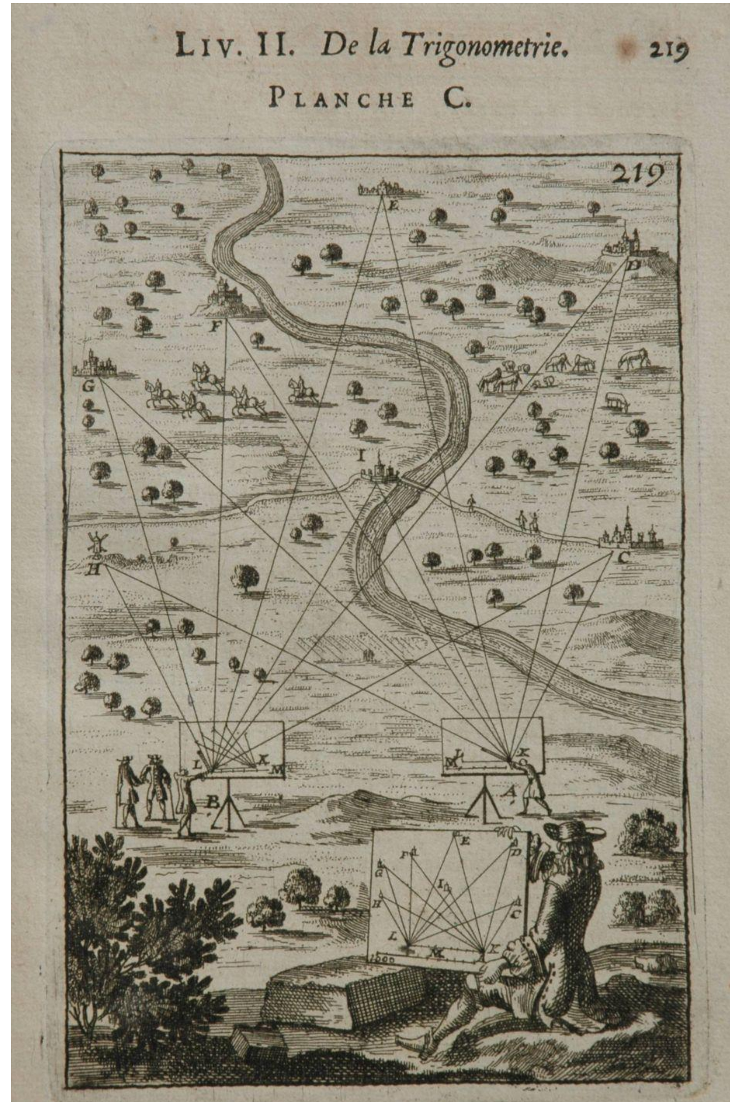
Affine span of (k+1) points: weighted barycentric equation

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

Key ideas:

- ~~tPCA, PGA: Look at data points from the mean (mean has to be unique)~~

- Triangulate from several reference: **locus of weighted means**



A. Manesson-Mallet. La géométrie Pratique, 1702

Barycentric subspaces and Affine span in Riemannian manifolds

Fréchet / Karcher barycentric subspaces (KBS / FBS)

- Absolute / local minima of weighted variance: $\sigma^2(x,\lambda) = \sum \lambda_i dist^2(x, x_i)$
- Also works in stratified spaces (e.g. trees) [LFM of Weyenberg, Nye]

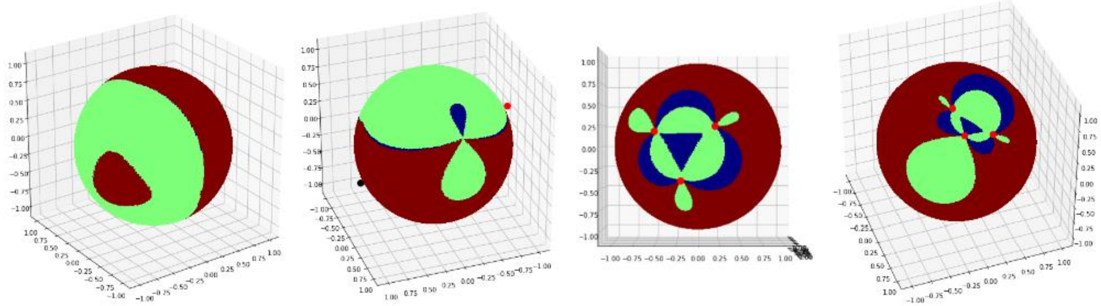
Exponential barycentric subspace and affine span

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

Properties (k+1 affinely independent reference points)

- BS are well defined in a neighborhood of reference points
- Local k-dim submanifold (det(H) ≠0), globally stratified space
- EBS = critical points of the weighted variance partitioned into a cell complex by the index of the Hessian (irruption of algebraic geometry)

[X.P. Annals of Statistics 2018]



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: $FL(x_0 \prec x_1 \prec \cdots \prec x_n)$

- Sequence of nested subspaces

$$Aff(x_0) \subset Aff(x_0, x_1) \subset \cdots Aff(x_0, \dots x_i) \subset \cdots Aff(x_0, \dots x_n) = M$$

Barycentric subspace analysis (BSA):

- Energy on flags: Accumulated Unexplained Variance
  → **optimal flags of subspaces in Euclidean spaces = PCA**

[X.P. Barycentric Subspace Analysis on Manifolds, Annals of Statistics 2018]

Robustness with L_p norms

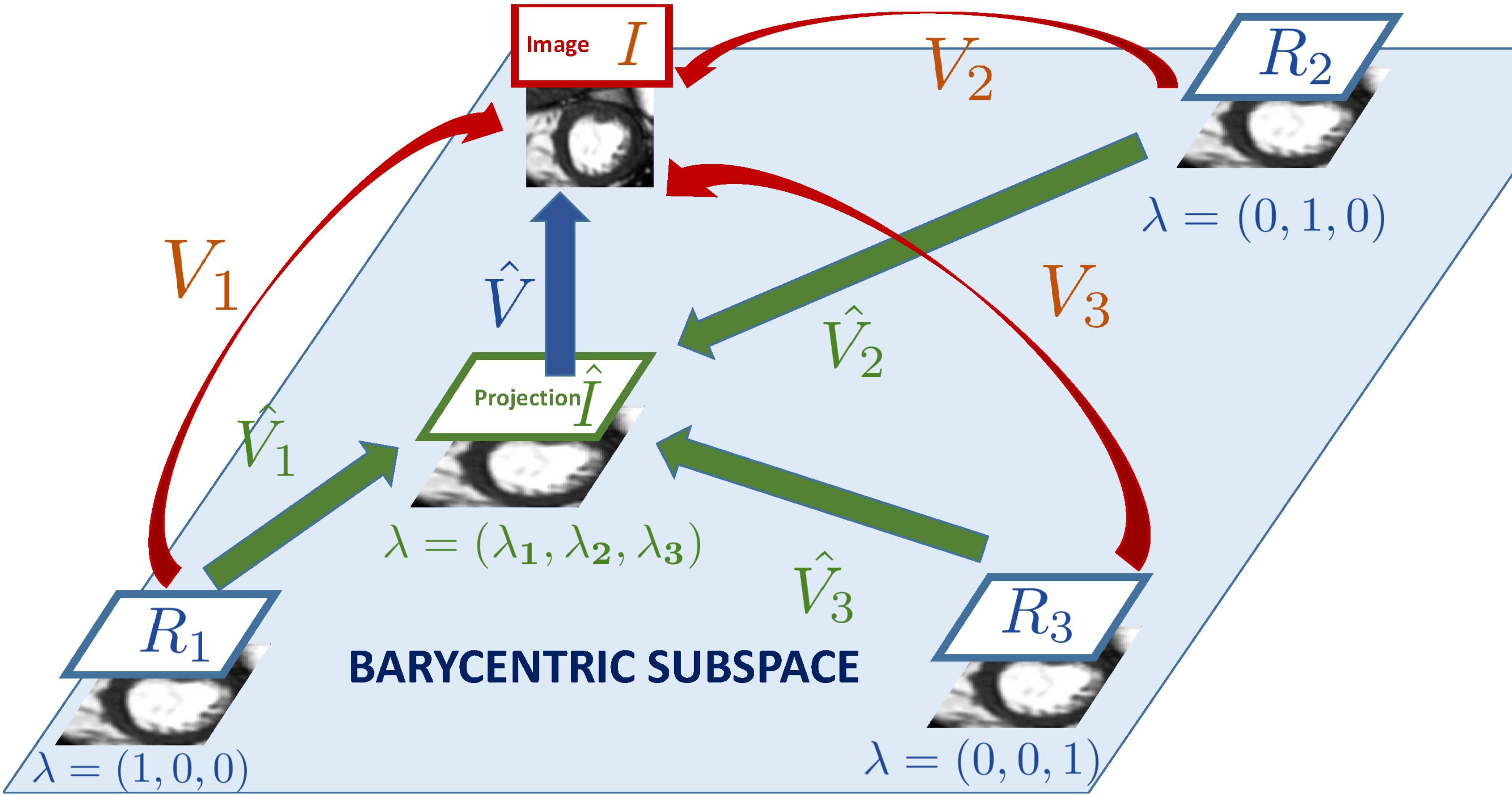
Affine spans is stable to p-norms

- $\sigma^p(x,\lambda) = \frac{1}{p}\sum\lambda_i dist^p(x,x_i)/\sum\lambda_i$
- Critical points of $\sigma^p(x,\lambda)$ are also critical points of $\sigma^2(x,\lambda')$ with $\lambda_i' = \lambda_i\, dist^{p-2}(x,x_i)$ (non-linear reparameterization of affine span)

Unexplained p-variance of residuals

- $2 < p \to +\infty$: more weight on the tail,
  at the limit: penalizes the maximal distance to subspace
- $0 < p < 2$: less weight on the tail of the residual errors: statistically robust estimation
  - Non-convex for p<1 even in Euclidean space
  - But sample-limited algorithms do not need gradient information

Application in Cardiac motion analysis

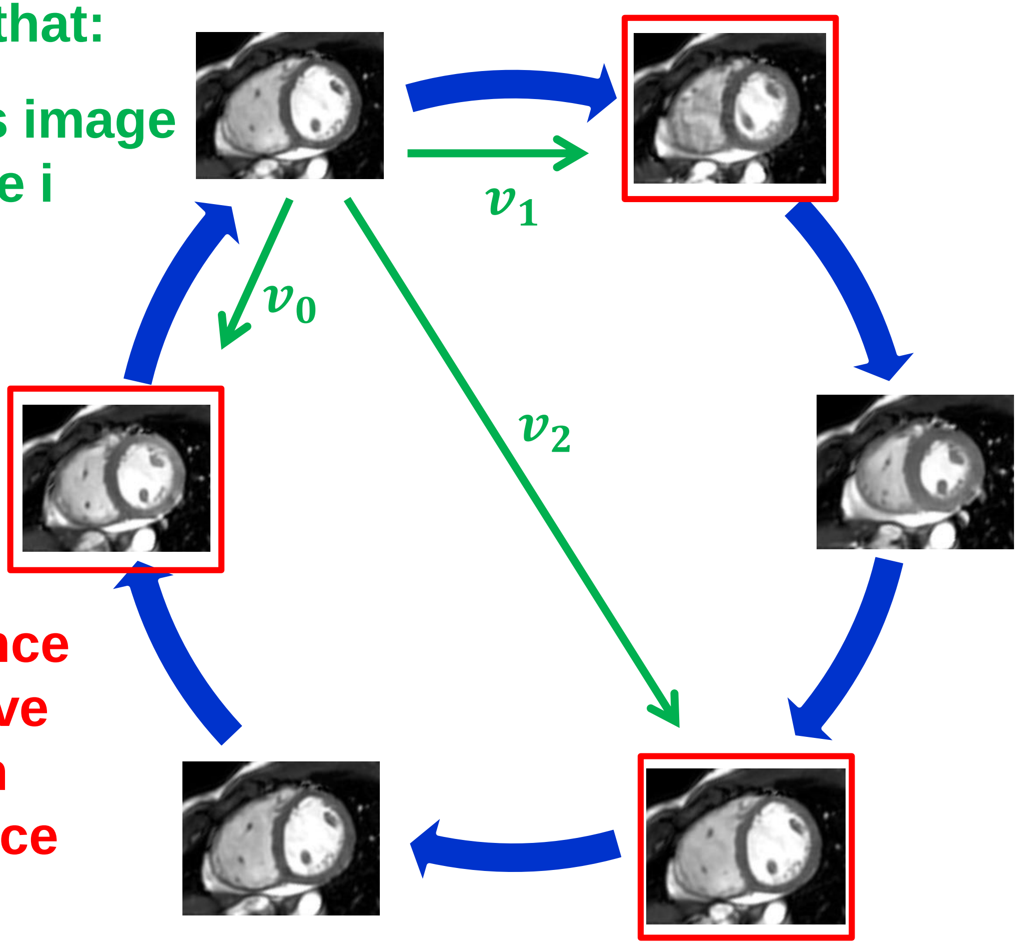


[Marc-Michel Rohé et al., MICCAI 2016, MedIA 45:1-12, 2018]

Application in Cardiac motion analysis

Find weights λ_i and SVFs v_i such that:

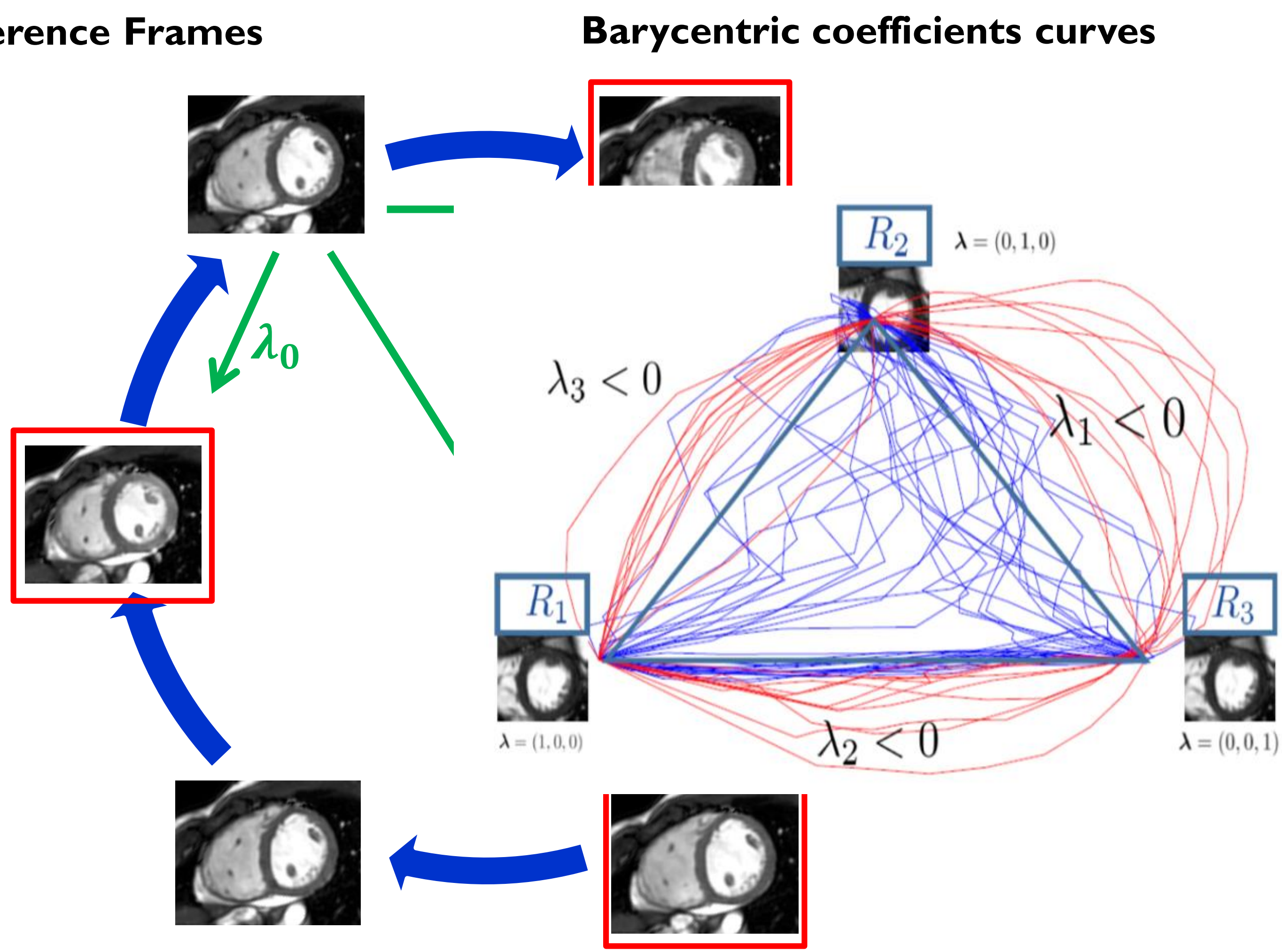
- v_i **registers image to reference i**
- $\sum_i \lambda_i v_i = 0$



Optimize reference images to achieve best registration over the sequence

[Marc-Michel Rohé et al., MICCAI 2016, MedIA 45:1-12, 2018]

Application in Cardiac motion analysis

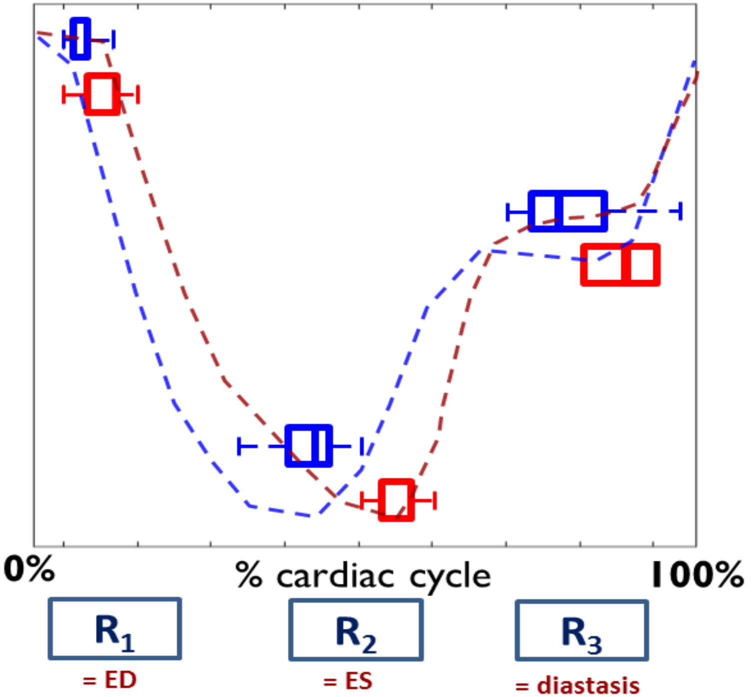


[Marc-Michel Rohé et al., MICCAI 2016, MedIA 45:1-12, 2018]

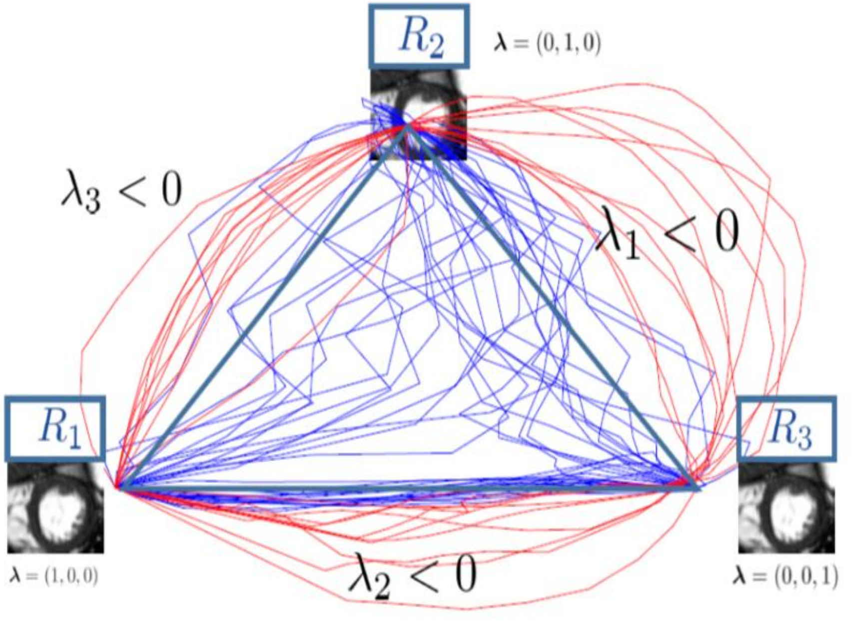
Cardiac Motion Signature

Low-dimensional representation of motion using:

Optimal Reference Frames



Barycentric coefficients curves



Dimension reduction from **+10M voxels** to **3 reference** frames + **60 coefficients**

Tested on **10 controls** [1] and **16 Tetralogy of Fallot** patients [2]

[1] Tobon-Gomez, C., et al.: Benchmarking framework for myocardial tracking and deformation algorithms: an open access database. Medical Image Analysis (2013)

[2] Mcleod K., et al.: Spatio-Temporal Tensor Decomposition of a Polyaffine Motion Model for a Better Analysis of Pathological Left Ventricular Dynamics. IEEE TMI (2015)

Take home messages

Natural subspaces in manifolds

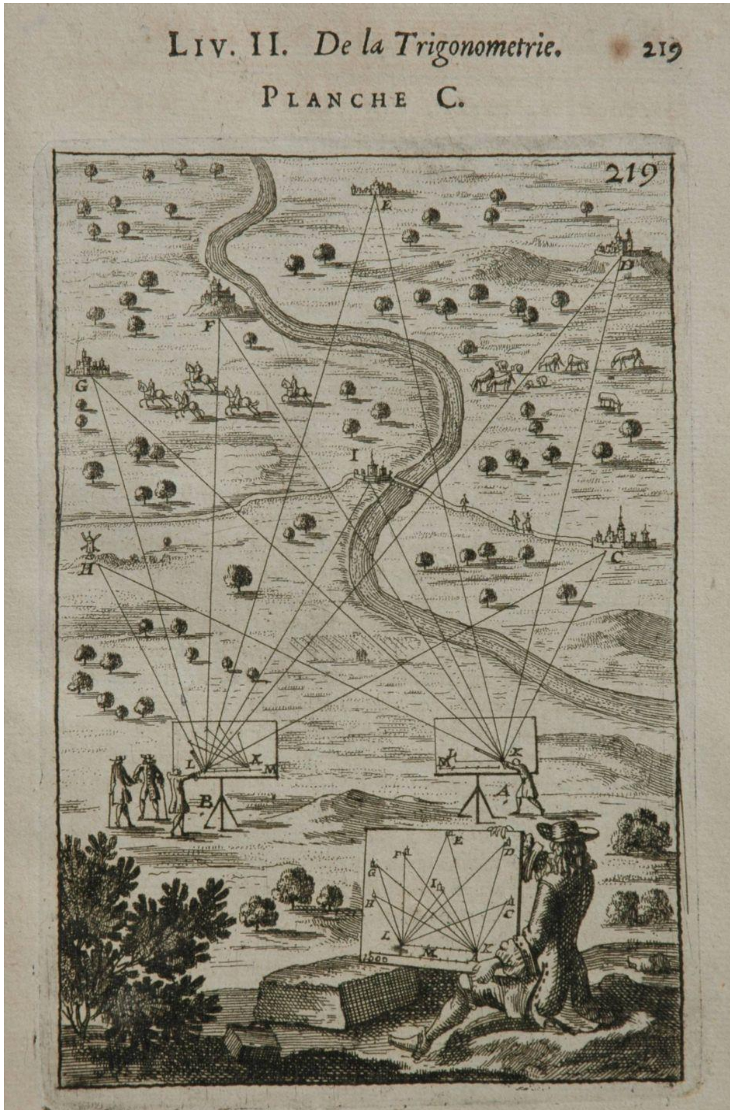
- PGA & Godesic subspaces:
  look at data points from the (unique) mean
- Barycentric subspaces:
  « triangulate » several reference points
  - Justification of multi-atlases?

Critical points (affine span) rather than minima (FBS/KBS)

- Barycentric coordinates need not be positive (convexity is a problem)
- Affine notion (more general than metric)
  - Generalization to Lie groups (SVFs)?

Natural flag structure for PCA

- Hierarchically embedded approximation subspaces to summarize / describe data



A. Manesson-Mallet. La géométrie Pratique, 1702

Outline

Statistics beyond the mean

Beyond the Riemannian metric: an affine setting

- The bi-invariant Cartan connection on Lie groups
- Extending statistics without a metric

Conclusions

Limits of the Riemannian Framework

Lie group: Smooth manifold with group structure

- Composition g o h and inversion g^{-1} are smooth
- Left and Right translation $L_g(f) = g \circ f$ $R_g(f) = f \circ g$
- Natural Riemannian metric choices using left OR right translation

No bi-invariant metric in general

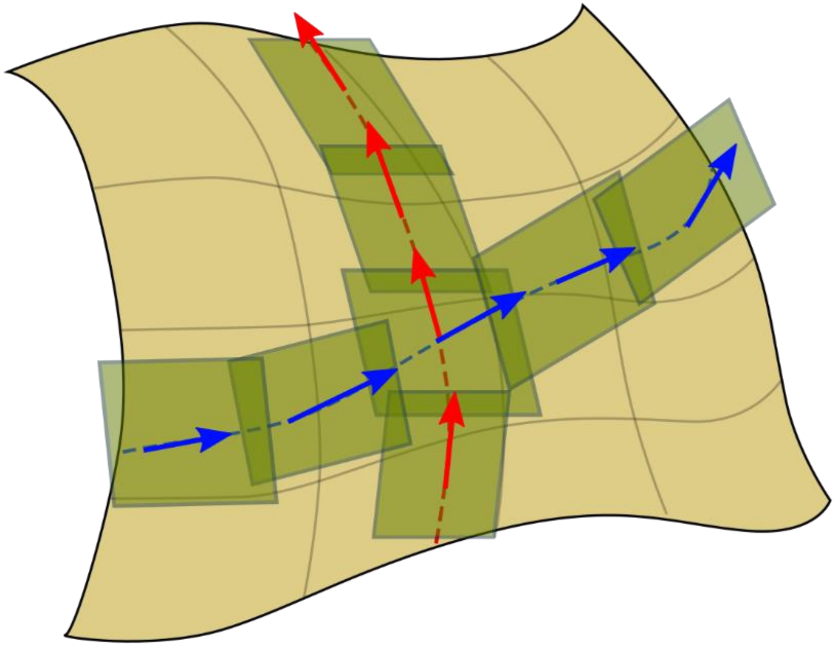
- **Incompatibility of the Fréchet mean with the group structure**
  - Left of right metric: different Fréchet means
  - The inverse of the mean is not the mean of the inverse
- Examples with simple 2D rigid transformations

- **Can we design a mean compatible with the group operations?**
- **Is there a more convenient non-Riemannian structure?**

Smooth affine connection spaces: Drop the metric, use connection to define geodesics

Affine Connection (infinitesimal parallel transport)

- Acceleration = derivative of the tangent vector along a curve
- Projection of a tangent space on a neighboring tangent space



Geodesics = straight lines

- Null acceleration: $\nabla_{\dot{\gamma}} \dot{\gamma} = 0$
- 2nd order differential equation: Normal coordinate system
- Local exp and log maps

[Lorenzi, Pennec. Geodesics, Parallel Transport & One-parameter Subgroups for Diffeomorphic Image Registration. Int. J. of Computer Vision, 105(2):111-127, 2013.]

Canonical Connections on Lie Groups

A unique Cartan-Schouten connection

- Bi-invariant and symmetric (no torsion)
- Geodesics through Id are one-parameter subgroups (group exponential)
  - Matrices : M(t) = A exp(t.V)
  - Diffeos : **translations of Stationary Velocity Fields (SVFs)**

Levi-Civita connection of a bi-invariant metric (if it exists)

- Continues to exists in the absence of such a metric (e.g. for rigid or affine transformations)

Symmetric space with central symmetry $S_\psi(\phi) = \psi \phi^{-1} \psi$

- Matrix geodesic symmetry: $S_A\big(M(t)\big) = A \exp(-tV) A^{-1} A = M(-t)$

[Lorenzi, Pennec. Geodesics, Parallel Transport & One-parameter Subgroups for Diffeomorphic Image Registration. Int. J. of Computer Vision, 105(2):111-127, 2013.]

Statistics on an affine connection space

~~Fréchet mean~~: exponential barycenters

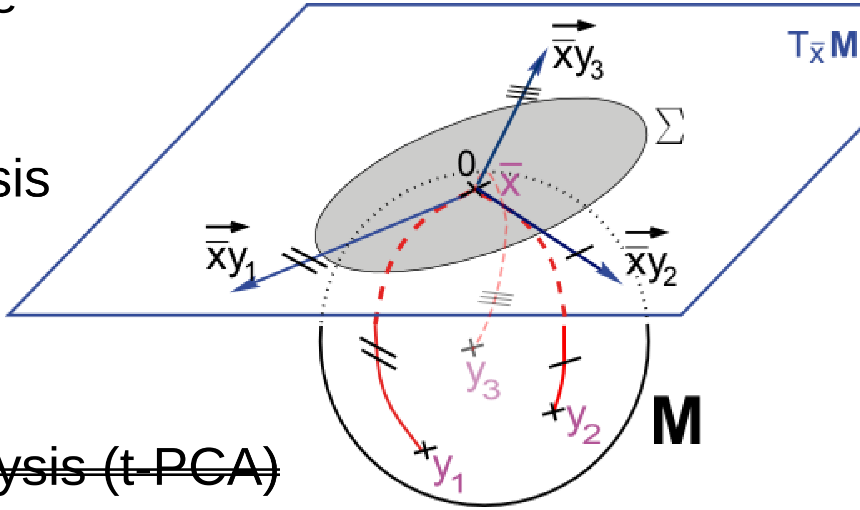
- $\sum_i Log_x(y_i) = 0$ [Emery, Mokobodzki 91, Corcuera, Kendall 99]
- Existence **local uniqueness** if local convexity [Arnaudon & Li, 2005]

Covariance matrix & higher order moments

- Defined as tensors in tangent space

$$\Sigma = \int Log_x(y) \otimes Log_x(y)\, \mu(dy)$$

- Matrix expression changes with basis



Other statistical tools

- Mahalanobis distance, chi[2] test
- ~~Tangent Principal Component Analysis (t-PCA)~~
- Independent Component Analysis (ICA)?

[XP & Arsigny, 2012, XP & Lorenzi, Beyond Riemannian Geometry, 2019]

Statistics on an affine connection space

For Cartan-Schouten connections [Pennec & Arsigny, 2012]

- Locus of points *x* such that $\sum Log(x^{-1}.y_i) = 0$
- Algorithm: fixed point iteration (**local convergence**)

$$x_{t+1} = x_t \circ Exp\left(\frac{1}{n}\sum Log(x_t^{-1}.y_i)\right)$$

- **Mean stable by left / right composition and inversion**

Matrix groups with no bi-invariant metric

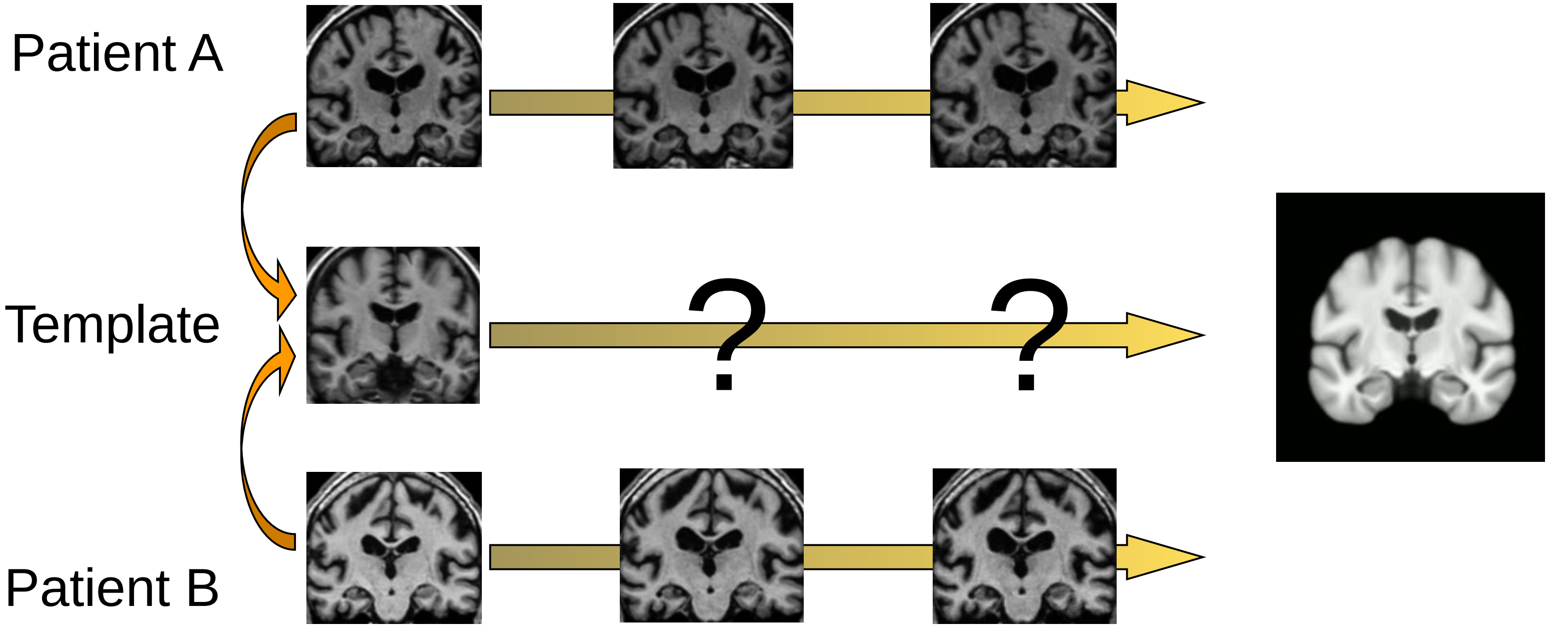
- Heisenberg group: bi-invariant mean is unique (conj. ok for solvable)
- Rigid-body transformations: uniqueness if unique mean rotation
- SU(n) and GL(n): log does not always exist (need 2 exp to cover)

[XP and V. Arsigny. Exponential Barycenters of the Canonical Cartan Connection and Invariant Means on Lie Groups. In Matrix Information Geometry. 2012]

The Stationnary Velocity Fields (SVF) framework for diffeomorphisms

- SVF framework for diffeomorphisms is algorithmically simple
- Compatible with “inverse-consistency” **[Lorenzi, XP. IJCV, 2013]**
- Vector statistics directly generalized to diffeomorphisms.
- **Exact parallel transport** using one step of pole ladder **[XP arxiv 1805.11436 2018]**

Longitudinal modeling of AD: 70 subjects extrapolated from 1 to 15 years



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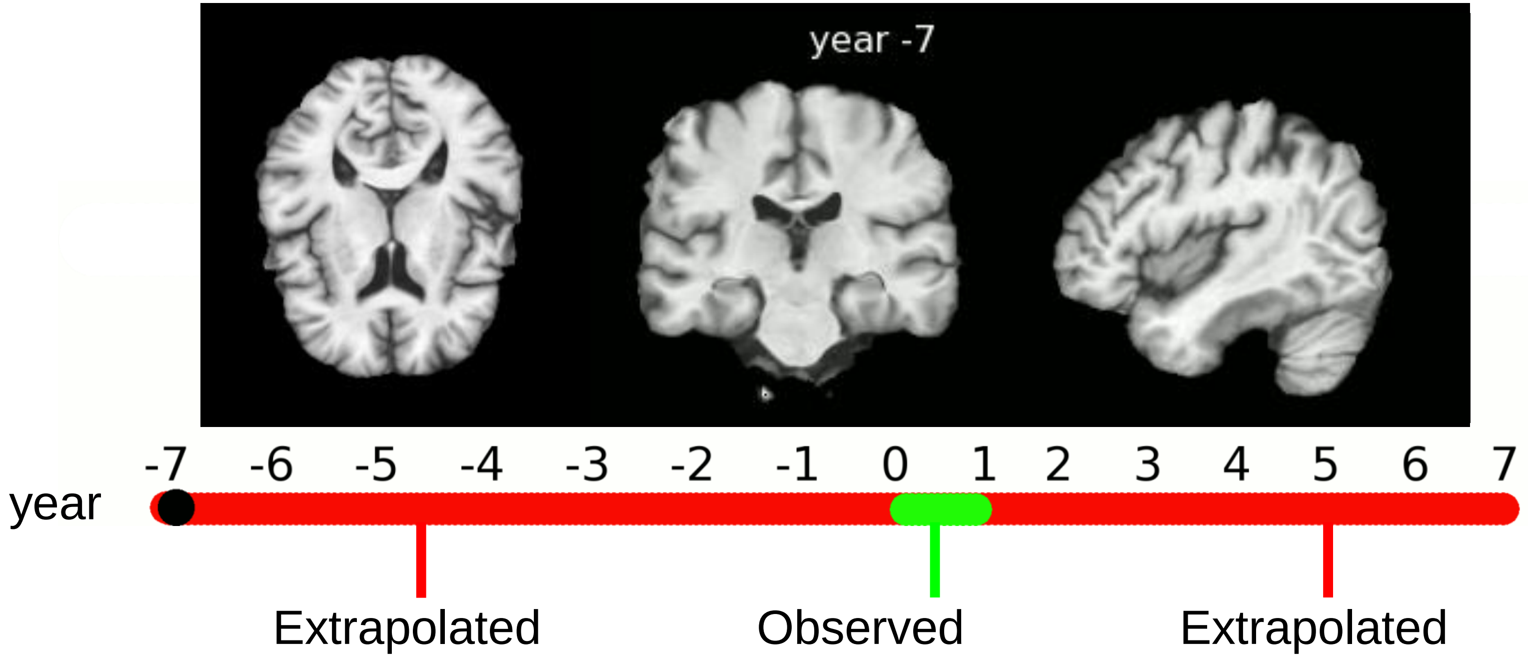


Cartan-Schouten Connections vs Riemannian metric

What is similar

- Standard differentiable geometric structure [curved space without torsion]
- Normal coordinate system with Exp_x et Log_x [finite dimension]

Limitations of the affine framework

- No metric to measure
- The exponential does always not cover the full group
  - Pathological examples close to identity in finite dimension
  - Similar limitations for the discrete Riemannian framework

What we gain

- No metric choice to justify
- A globally invariant structure invariant by composition & inversion
- Simple geodesics, efficient computations (stationarity, group exponential)
- **A global symmetry that may simplify algorithms**

Outline

Statistics beyond the mean

Beyond the Riemannian metric: an affine setting

Conclusions:

Beyond Riemannian and affine geometries?

Pushing the frontiers of Geometric Statistics

Beyond the Riemannian / metric structure

- Riemannian manifolds, Non-Positively Curved (NPC) metric spaces
- Towards **Affine connection, Quotient, Stratified spaces**

Beyond the mean and unimodal concentrated laws

- **Flags (nested sequences) of subspace in manifolds**
- **Non Gaussian statistical models within subspaces?**

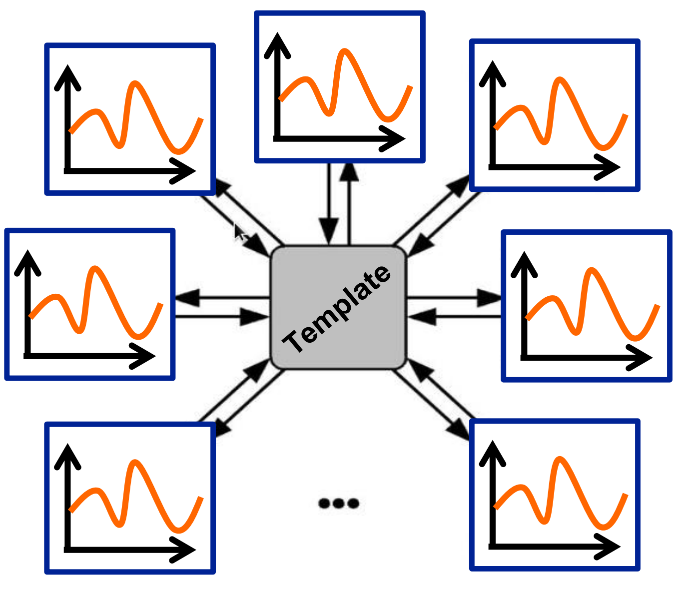
Unify statistical estimation theory

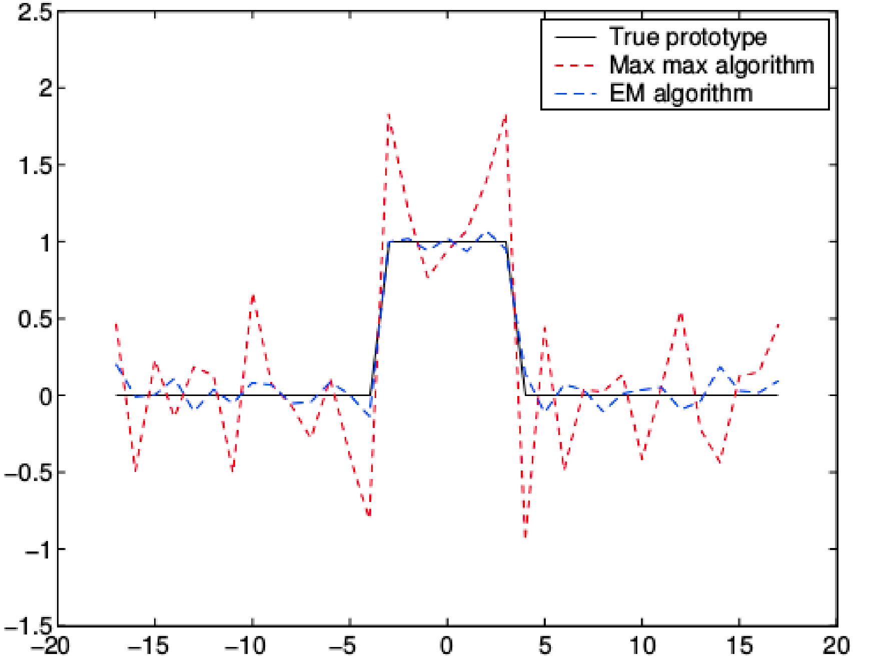
- Explore influence of **curvature, singularities** (borders, corners, stratifications) on non-asymptotic estimation theory

Quotient spaces

Functions/Images modulo time/space parameterization

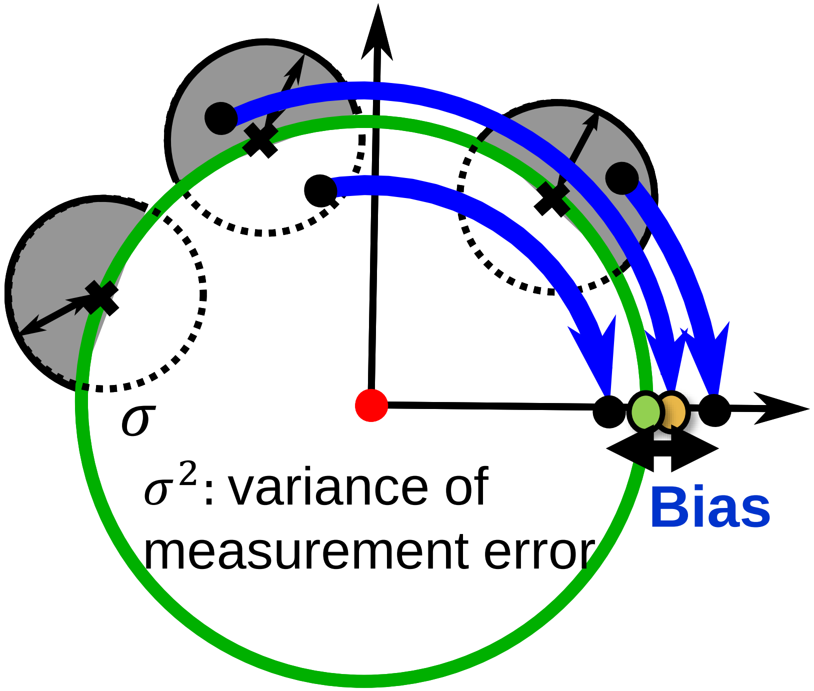
- Amplitude and phase discrimination problem





[Allassoniere, Amit, Trouvé, 2005],
Example by Loic Devillier, IPMI 2017

Noise in top space = Bias in quotient spaces



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

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

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

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

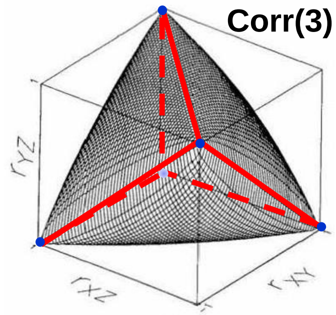
Extension to Hilbert of ∞-dim: bias for $\sigma > 0$, asymptotic for $\sigma \to \infty$,
[Devilliers, Allasonnière, Trouvé and XP. SIIMS 2017, Entropy, 2017]

→ Estimated atlas is topologically more complex than should be

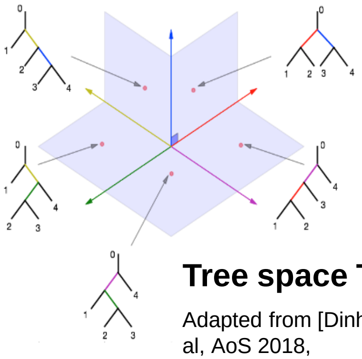
Towards non-smooth spaces

Stratified spaces

- Correlation matrices
  - Positive semi definite (PSD) matrices with unit diagonal [Grubisic and Pietersz, 2004]
- Orthant spaces (phylogenetic trees)
  - BHV tree space [Billera Holmes Voigt, Adv Appl Math, 2001] [Nye AOS 2011] [Feragen 2013] [Barden & Le, 2017]



Adapted from [Rousseeuw and Molenberghs, 1994].

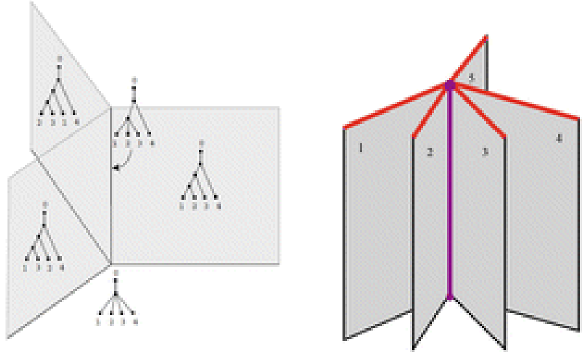


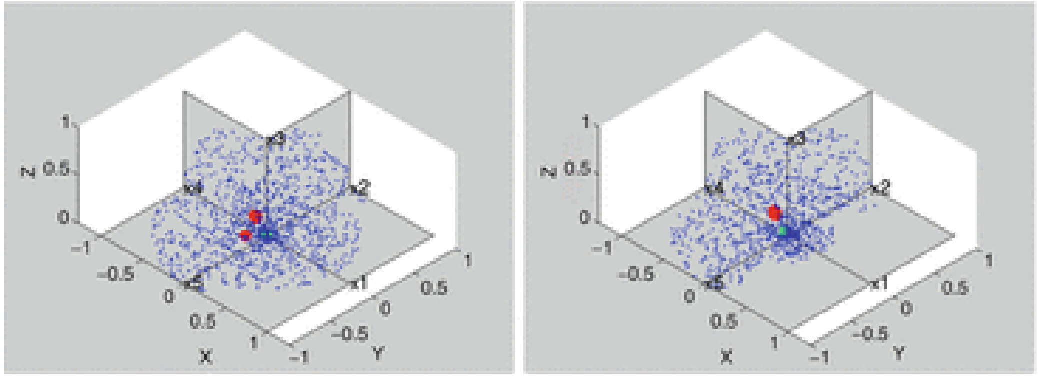
Tree space T4

Adapted from [Dinh et al, AoS 2018,

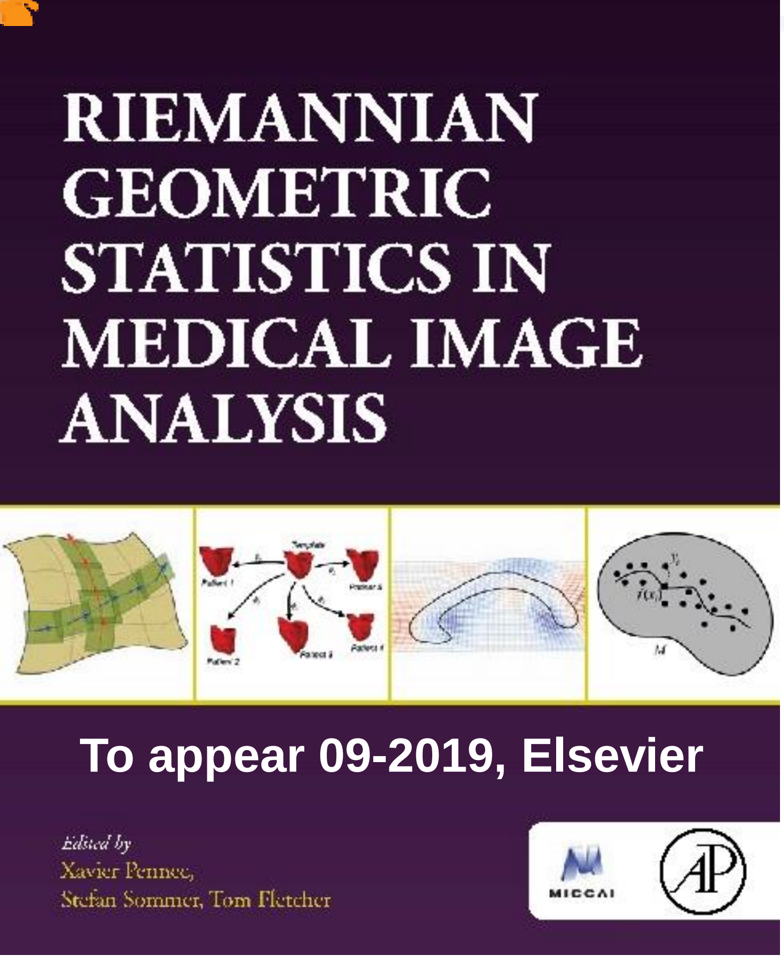
Can we explain non standard statistical results?

- **Sticky mean** [Hotz et al 2013] [Barden & Le 2017], **repulsive mean** [Miolane 2017]
- **Faster convergence rate with #sample in NPC spaces** [Basrak, 2010]





[Ellingson et al, Topics in Nonparametric Statistics, 2014]



Part 1: Foundations

- 1:Riemannian geometry [Sommer, Fetcher, Pennec]
- 2: Statistics on manifolds [Fletcher]
- 3: Manifold-valued image processing with SPD matrices [Pennec]
- 4: Riemannian Geometry on Shapes and Diffeomorphisms [Marsland, Sommer]
- 5: Beyond Riemannian: the affine connection setting for transformation groups [Pennec, Lorenzi]

Part 2: Statistics on Manifolds and Shape Spaces

- 6: Object Shape Representation via Skeletal Models (s-reps) and Statistical Analysis [Pizer, Maron]
- 7: Inductive Fréchet Mean Computation on S(n) and SO(n) with Applications [Chakraborty, Vemuri]
- 8: Statistics in stratified spaces [Ferage, Nye]
- 9: Bias in quotient space and its correction [Miolane, Devilier,Pennec]
- 10: Probabilistic Approaches to Statistics on Manifolds: Stochastic Processes, Transition Distributions, and Fiber Bundle Geometry [Sommer]
- 11: Elastic Shape Analysis, Square-Root Representations and Their Inverses [Zhang, Klassen, Srivastava]

Part 3: Deformations, Diffeomorphisms and their Applications

- 13: Geometric RKHS models for handling curves and surfaces in Computational Anatomy : currents, varifolds, f-shapes, normal cycles [Charlie, Charon, Glaunes, Gori, Roussillon]
- 14: A Discretize-Optimize Approach for LDDMM Registration [Polzin, Niethammer, Vialad, Modezitski]
- 15: Spatially varying metrics in the LDDMM framework [Vialard, Risser]
- 16: Low-dimensional Shape Analysis In the Space of Diffeomorphisms [Zhang, Fleche, Wells, Golland]
- 17: Diffeomorphic density matching, Bauer, Modin, Joshi]

Thank you for your attention

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    Warning: change of denomination since this paper: EBS →affine span
  - **Barycentric Subspaces Analysis on Spheres** Mathematical Foundations of Computational Anatomy (MFCA'15), Oct 2015, Munich, Germany. pp.71-82, 2015. https://hal.inria.fr/hal-01203815
- **Sample-limited L p Barycentric Subspace Analysis on Constant Curvature Spaces.** X.P. Geometric Sciences of Information (GSI 2017), Nov 2017, Paris, France. LNCS 10589, pp.20-28, 2017.
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- Xavier Pennec, Pierre Fillard, and Nicholas Ayache. A Riemannian Framework for Tensor Computing. International Journal of Computer Vision, 66(1):41-66, Jan. 2006. http://www.inria.fr/sophia/asclepios/Publications/Xavier.Pennec/Pennec.IJCV05.pdf

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