Xavier Pennec

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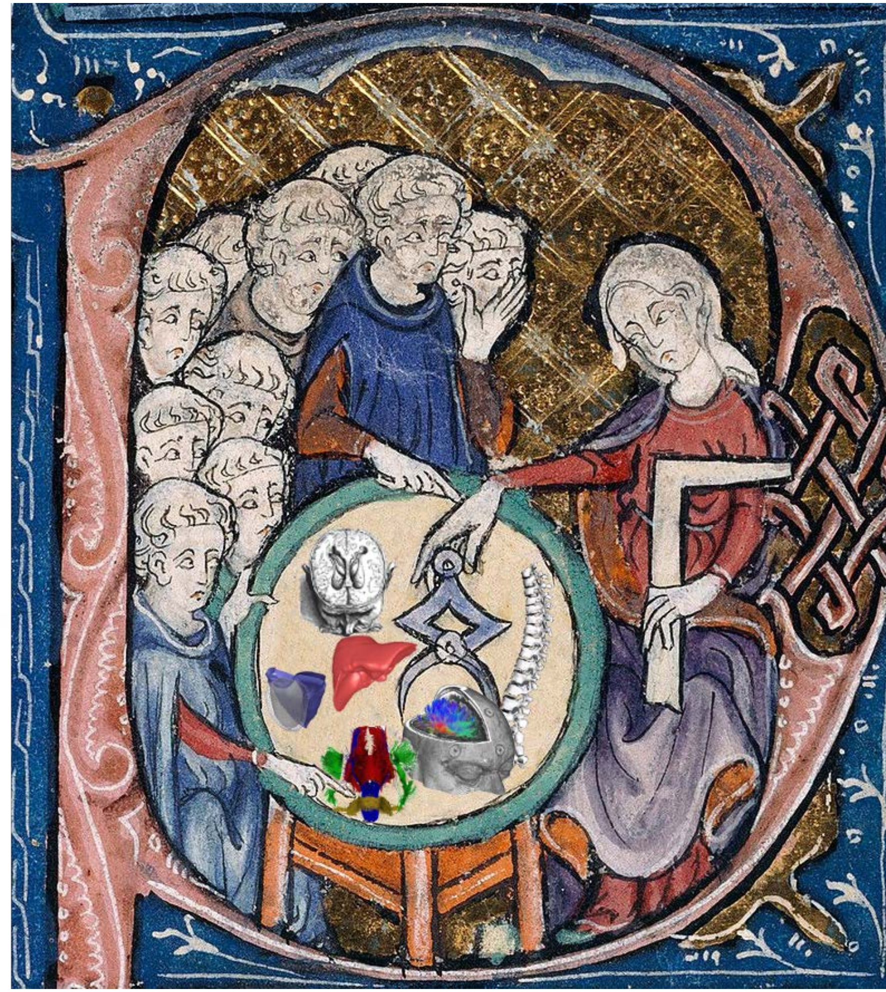


Freely adapted from "Women teaching geometry", in Adelard of Bath translation of Euclid's elements, 1310.

Geometric Statistics

Mathematical foundations and applications in computational anatomy

3/ Advanced Stats: empirical estimation and generalized PCA

Geometric Statistics workshop 09/2019

Geometric Statistics: Mathematical foundations and applications in computational anatomy

Intrinsic Statistics on Riemannian Manifolds

Metric and Affine Geometric Settings for Lie Groups

Advances Statistics: CLT & PCA

- Estimation of the empirical Fréchet mean & CLT
- Principal component analysis in manifolds
- Natural subspaces in manifolds: barycentric subspaces
- Rephrasing PCA with flags of subspaces

Several definitions of the mean

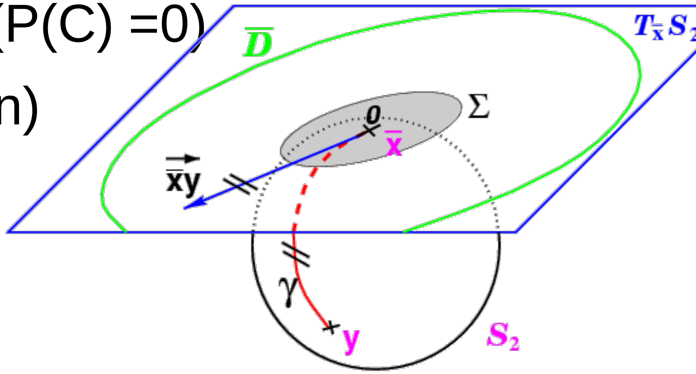
Tensor moments of a random point on M

- $\mathfrak{M}_1(x) = \int_M \overrightarrow{xz}\, dP(z)$ Tangent mean: (0,1) tensor field
- $\mathfrak{M}_2(x) = \int_M \overrightarrow{xz} \otimes \overrightarrow{xz}\, dP(z)$ 2nd moment: (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
- $\sigma^2(x) = Tr_g\big(\mathfrak{M}_2(x)\big) = \int_M dist^2(x,z)\, dP(z)$ **Mean quadratic deviation**

Mean value = optimum of the variance

- **Frechet mean** [1944] = (global) minima of p-deviation (includes median)
- **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

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

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

- [Bonnabel IEE TAC 58(9) 2013]
- [Arnaudon & Miclo, Stoch. Proc. & App. 124, 2014]

Asymptotic behavior of the mean

Uniqueness of p-means with convex support

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

- Non-positively curved metric spaces (Aleksandrov): OK [Gromov, Sturm]
- Positive curvature: [Karcher 77 & Kendall 89] concentration conditions: Support in a regular geodesic ball of radius $r < r^* = \frac{1}{2}\min(inj(M), \pi/\sqrt{\kappa})$

Bhattacharya-Patrangenaru CLT [BP 2005, B&B 2008]

- Under suitable concentration conditions [KKC], for IID n-samples:
  - $\bar{x}_n \rightarrow \bar{x}$ *(consistency of empirical mean)*
  - $\sqrt{n}\, log_{\bar{x}}(\bar{x}_n) \rightarrow N(0, 4\bar{H}^{-1}\,\Sigma\,\bar{H}^{-1})$ *if* $\bar{H} = \int_M Hess_{\bar{x}}\left(d^2(y, \bar{x})\right) \mu(dy)$ *invertible*
- Problems for larger supports [Huckemann & Eltzner, H. Le]

Behavior in high concentration conditions?

- Interpretation of the mean Hessian?
- What happens for a small sample size (non-asymptotic behavior)?
- Can we extend results to affine connection spaces?

Concentration assumptions

- Uniqueness of the mean, support of diameter < ε

Riemannian manifold: Karcher & Kendall Concentr. Cond.

- $\mathrm{Supp}(\mu) \subset B(x,r)$ with $\mathrm{r} < \frac{1}{2}\, inj(x)$
- $\sup_{x \in B(x,r)} \kappa(x) < \pi^2/(4r)^2$

Affine connection spaces: Arnaudon & Li convexity cond.

- $\rho: M \times M \rightarrow R^+$ separating function
  - Separability: $\rho(x,y) = 0 \Leftrightarrow x = y$
  - Convexity along geodesic: $\rho(\gamma_1(t), \gamma_2(t)): R \rightarrow R^+ \; convex$
- p-convex geometry: $\mathrm{c\,dist^p(x,y)} \leq \rho(x,y) \leq C\, dist^p(x,y)$
- Uniqueness of exponential barycenter (compact support)

Taylor expansion in manifolds

The mean is an exponential barycenter

- The zero of the tangent mean field (Brewin Taylor expansion)

$$\mathfrak{M}_1(x) = \int_M \log_x(z)\, \mu(dz) \text{ has a zero at } \bar{x}.$$

Lots of additional terms in higher order derivatives since the vector field expression at $x_v = \exp_x(v)$ in a normal coordinates at x is modulated by $\mathrm{D}\exp_x(v)$.

- The zero of a mapping of vector spaces: the recenterd mean field

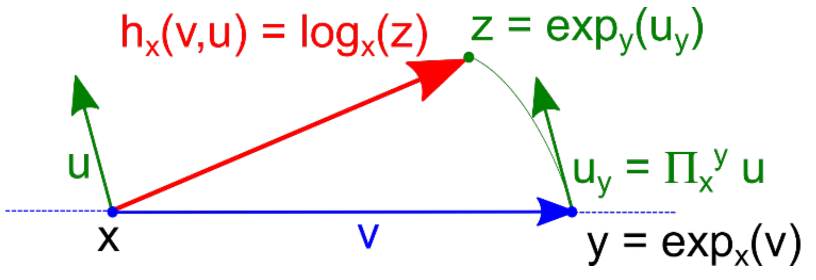
$$N_x(v) = \Pi_{x_v}^{x} \mathfrak{M}_1(\exp_x(v)) = \int_M \Pi_{x_v}^{x} \log_{x_v}(y)\, \mu(dy)$$

$\bar{x}$ is a Fréchet mean iff $N_x(v)$ has a zero at $\mathrm{v} = \log_x(\bar{x})$

Goal: compute a series expansion w.r.t. v

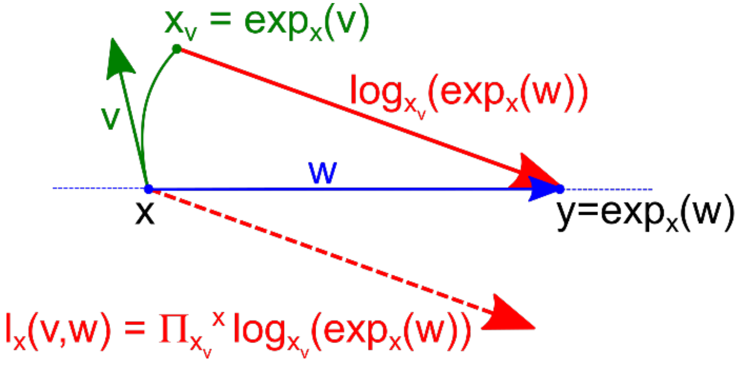
Taylor expansion in manifolds

Gavrilov's double exponential series (2006):



$$h_x(v,u) = \log_x(\Pi_x^{\exp_x(v)} u)$$
$$= v + u + \frac{1}{6} R(u,v)v + \frac{1}{3} R(u,v)u$$
$$+ \frac{1}{24} \nabla_v R(u,v)(2v + 5u)$$
$$+ \frac{1}{24} \nabla_u R(u,v)(v + 2u) + O(5)$$

Neighboring log expansion (new)



$$l_x(v,w) = \Pi_{x_v}^x \log_{x_v}(\exp_x(w))$$
$$= w - v + \frac{1}{6} R(w,v)(v - 2w)$$
$$+ \frac{1}{24} \nabla_v R(w,v)(2v - 3w)$$
$$+ \frac{1}{24} \nabla_w R(w,v)(v - 2w) + O(5)$$

Taylor expansion of recentered mean map

$$\mathfrak{N}_x^{\mu}(v) = \mathfrak{M}_1 - v + \frac{1}{6}R(\mathfrak{M}_1, v)v - \frac{1}{3}R(\bullet, v)\bullet : \mathfrak{M}_2 + \frac{1}{12}(\nabla_v R)(\mathfrak{M}_1, v)v$$
$$+ \frac{1}{24}(\nabla_\bullet R)(\bullet, v)v : \mathfrak{M}_2 - \frac{1}{8}(\nabla_v R)(\bullet, v)\bullet : \mathfrak{M}_2 - \frac{1}{12}(\nabla_\bullet R)(\bullet, v)\bullet : \mathfrak{M}_3 + O(\varepsilon^5)$$

Solving for the value $v = \log_x(\bar{x})$ that zeros the polynomial

$$\log_x(\bar{x}) = \mathfrak{M}_1 - \frac{1}{3}R(\bullet, \mathfrak{M}_1)\bullet : \mathfrak{M}_2 - \frac{1}{24}\nabla_\bullet R(\bullet, \mathfrak{M}_1)\mathfrak{M}_1 : \mathfrak{M}_2$$
$$- \frac{1}{8}\nabla_{\mathfrak{M}_1} R(\bullet, \mathfrak{M}_1)\bullet : \mathfrak{M}_2 - \frac{1}{12}\nabla_\bullet R(\bullet, \mathfrak{M}_1)\bullet : \mathfrak{M}_3 + O(\epsilon^5).$$

For an empirical an n-sample $\mathbf{X_n} = \frac{1}{n}\sum_i \delta_{x_i}$

$$\log_x(\bar{x}_n) = \mathfrak{X}_1^n - \frac{1}{3}R(\bullet, \mathfrak{X}_1^n)\bullet : \mathfrak{X}_2^n + \frac{1}{24}\nabla_\bullet R(\bullet, \mathfrak{X}_1^n)\mathfrak{X}_1^n : \mathfrak{X}_2^n$$
$$- \frac{1}{8}\nabla_{\mathfrak{X}_1^n} R(\bullet, \mathfrak{X}_1^n)\bullet : \mathfrak{X}_2^n - \frac{1}{12}\nabla_\bullet R(\bullet, \mathfrak{X}_1^n)\bullet : \mathfrak{X}_3^n + O(\epsilon^5).$$

Compute the expectation for a random n-sample?

Non-Asymptotic behavior of empirical means

Expectation of product of empirical moments

- $\mathbf{E}[\mathfrak{X}_k^n(x)] = \mathfrak{M}_k(x)$
- $\mathbf{E}\left[\mathfrak{X}_p^n \otimes \mathfrak{X}_q^n\right] = \frac{n-1}{n} \mathfrak{M}_{p+q} \otimes \mathfrak{M}_{p+q} + \frac{1}{n} \mathfrak{M}_{p+q}$
- Etc...

First Moment of the empirical mean

$$\begin{aligned}
\mathrm{E}\left[\, \log_x(\bar{x}_n) \,\right] &= \mathfrak{M}_1 - \frac{n-1}{3n} R(\bullet, \mathfrak{M}_1)\bullet \, \vdots \, \mathfrak{M}_2 \\
&+ \frac{(n-1)(n-2)}{24n^2} \left(\nabla_\bullet R(\bullet, \mathfrak{M}_1)\mathfrak{M}_1 \, \vdots \, \mathfrak{M}_2 - 3\nabla_{\mathfrak{M}_1} R(\bullet, \mathfrak{M}_1)\bullet \, \vdots \, \mathfrak{M}_2 \right) \\
&+ \frac{(n-1)}{12n^2} \left(2\nabla_\circ R(\circ, \bullet)\bullet \, \vdots \, \mathfrak{M}_2 \, \mathring{\vdots} \, \mathfrak{M}_2 - (1+n)\nabla_\bullet R(\bullet, \mathfrak{M}_1)\bullet \, \vdots \, \mathfrak{M}_3 \right) + O(\epsilon^5).
\end{aligned}$$

At the population mean:

$$\mathrm{E}\left[\, \log_{\bar{x}}(\bar{x}_n) \,\right] = \frac{(n-1)}{6n^2} \nabla_\bullet R(\bullet, \circ)\circ \, \vdots \, \mathfrak{M}_2 \, \mathring{\vdots} \, \mathfrak{M}_2 + O(\epsilon^5).$$

Non-Asymptotic behavior of empirical means

Second Moment of the empirical mean a the pop. mean:

$$\mathbf{E}\left[\,\log_{\bar{x}}(\bar{x}_n)\otimes\log_{\bar{x}}(\bar{x}_n)\,\right]=\frac{1}{n}\mathfrak{M}_2-\frac{(n-1)}{3n^2}\mathfrak{M}_2 \mathbin{\overset{\circ}{\circ}} \left(\circ\otimes R(\bullet,\circ)\bullet+R(\bullet,\circ)\bullet\otimes\circ\right) \mathbin{\overset{\bullet}{\bullet}} \mathfrak{M}_2+O(\epsilon^5).$$

In coordinates:

$$\begin{aligned} Bias(\bar{x}_n)^a &= \tfrac{1}{6n}\left(1-\tfrac{1}{n}\right)\nabla_b R^a_{cde}\mathfrak{M}_2^{ce}\mathfrak{M}_2^{bd}+O\left(\epsilon^5\right) \\ Cov(\bar{x}_n)^{ab} &= \tfrac{1}{n}\left(\mathfrak{M}_2^{ab}-\tfrac{1}{3}\left(1-\tfrac{1}{n}\right)\mathfrak{M}_2^{cd}\left(\mathfrak{M}_2^{ae}R^b_{cde}+R^a_{cde}\mathfrak{M}_2^{be}\right)\right)+O\left(\epsilon^5\right). \end{aligned}$$

Non-Asymptotic behavior of empirical means

Moments of the Fréchet mean of a n-sample

- **Unexpected bias** in 1/n on empirical mean (**gradient of curvature-cov.**)

$$\mathbf{bias}(\bar{x}_n) = \boldsymbol{E}\left(log_{\bar{x}}(\bar{x}_n)\right) = \frac{\mathbf{1}}{\boldsymbol{6n}}\left(\mathfrak{M}_2 : \nabla \boldsymbol{R} : \mathfrak{M}_2\right) + O(\epsilon^5, 1/n^2)$$

- **Concentration rate** modulated by the **curvature-covariance**:

$$\boldsymbol{Cov}(\bar{x}_n) = \boldsymbol{E}\left(log_{\bar{x}}(\bar{x}_n) \otimes log_{\bar{x}}(\bar{x}_n)\right) = \frac{\mathbf{1}}{\boldsymbol{n}}\mathfrak{M}_2 + \frac{\mathbf{1}}{\boldsymbol{3n}}\mathfrak{M}_2 : \boldsymbol{R} : \mathfrak{M}_2 + O(\epsilon^5, 1/n^2)$$

  - **Asymptotically infinitely fast** CV for negative curvature
  - **No convergence (LLN fails)** at the limit of KKC condition

[XP, Curvature effects on the empirical mean in Manifolds 2019, arXiv:1906.07418]

Comparison with the BP CLT

Bhattacharya-Patrangenaru CLT [BP 2005, B&B 2008]

- Under suitable concentration conditions, for IID n-samples:
  - $\bar{x}_n \to \bar{x}$ *(consistency of empirical mean)*
  - $\sqrt{n}\, log_{\bar{x}}(\bar{x}_n) \to N(0, 4\bar{H}^{-1}\, \Sigma\, \bar{H}^{-1})$ *if* $\bar{H} = \int_M Hess_{\bar{x}}\big(\, d^2(y,\bar{x})\big)\, \mu(dy)$ *invertible*

Hessian: $\frac{1}{2}\bar{H} = Id + \frac{1}{3} R : \mathfrak{M}_2 + \frac{1}{12} \nabla \mathrm{R} : \mathfrak{M}_3 + O(\epsilon^4, 1/n^2)$

$$4[\bar{H}^{(-1)}\mathfrak{M}_2\bar{H}^{(-1)}]^{ab} = 4[\bar{H}^{(-1)}]^a_c[\mathfrak{M}_2]^{cd}[\bar{H}^{(-1)}]^b_d = \mathfrak{M}_2^{ab} - \frac{1}{3}\mathfrak{M}_2^{ef}\left(R^a_{efc}\mathfrak{M}_2^{cb} + \mathfrak{M}_2^{ad}R^b_{efd}\right) + O(\varepsilon^5),$$

Same limiting expansion for large n

Isotropic distribution in constant curvature spaces

- Symmetric spaces: no bias
- Variance is modulated w.r.t. Euclidean: $Var(\bar{x}_n) = \alpha \frac{\sigma^2}{n}$

High concentration expansion

- $\alpha = 1 + \frac{2}{3}\left(1 - \frac{1}{d}\right)\left(1 - \frac{1}{n}\right)\kappa\sigma^2 + O(\epsilon^5)$

Closed form for asymptotic BP-CLT expansion

$$\frac{1}{2} H_x(y) = uu^\top + h(\kappa\theta^2)(\mathrm{Id} - uu^\top) \qquad \text{with} \qquad h(t) = \sqrt{t}\cot(\sqrt{t})$$

- $\alpha = \left(\frac{1}{d} + \left(1 - \frac{1}{d}\right)\bar{h}\right)^{-2} + O(n^{-2})$

$$\bar{h} = \mathbf{E}\left[\, h(\kappa \operatorname{dist}(\bar{x}, .)^2)\,\right] = \int_{\mathcal{M}} h(\kappa(\operatorname{dist}(\bar{x}, y)^2)\, \mu(dy).$$

Isotropic distribution in constant curvature spaces

- Variance is modulated w.r.t. Euclidean: $Var(\bar{x}_n) = \alpha \frac{\sigma^2}{n}$

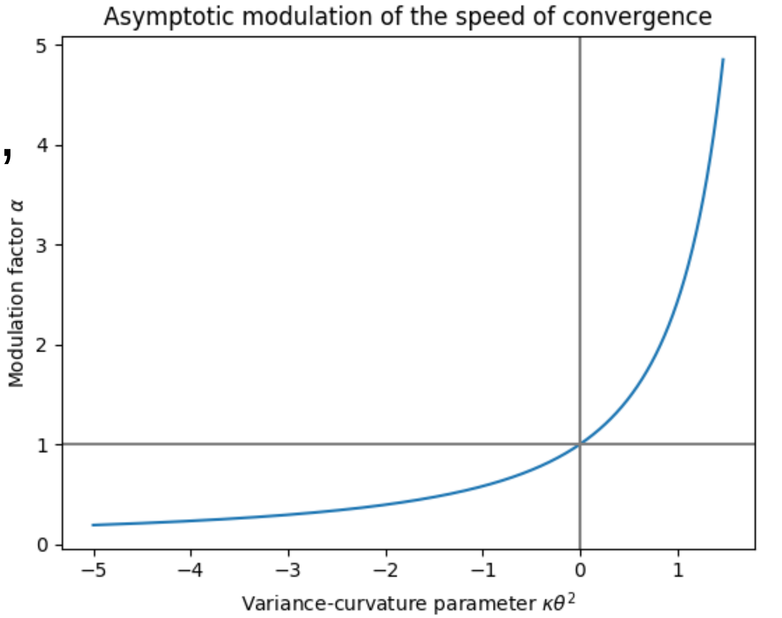
)

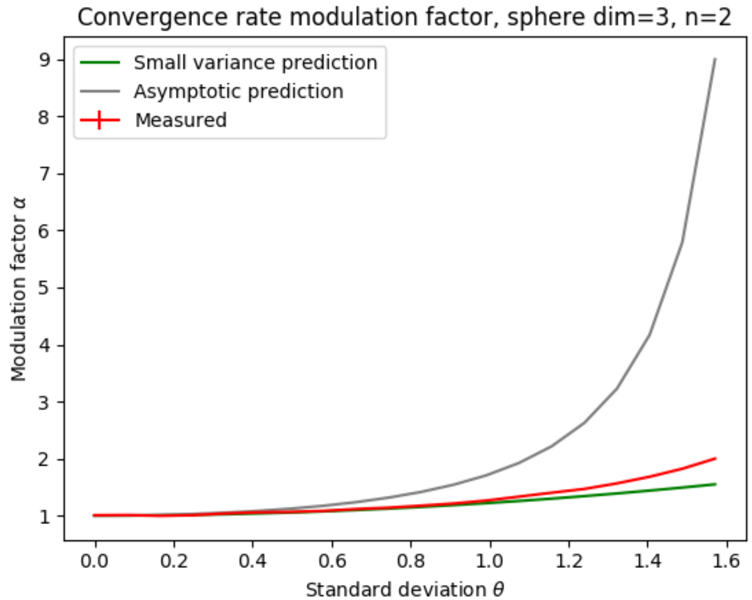
Asymptotic BP-CLT expansion

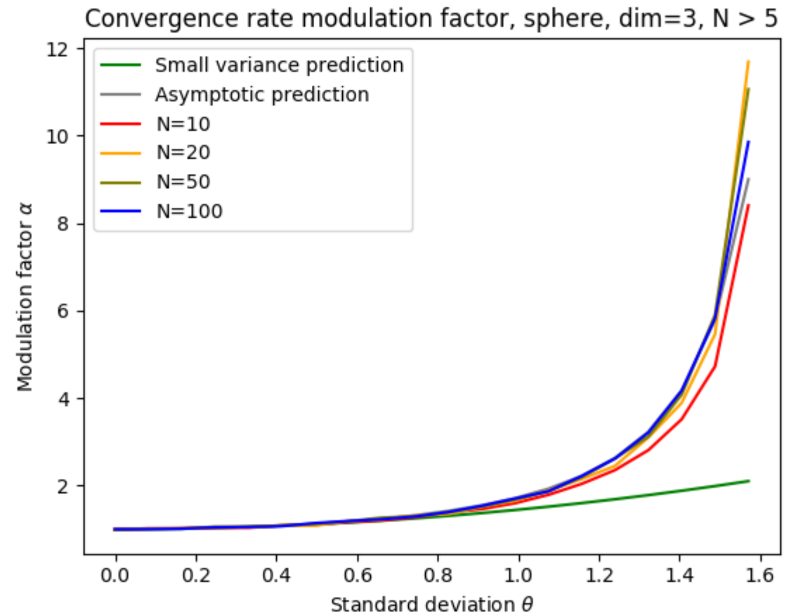
- $\alpha = \left(\frac{1}{d} + \left(1 - \frac{1}{d}\right)\bar{h}\right)^{-2} + O(n^{-2})$

Archetypal modulation factor

- Uniform distrib on $S(\bar{x}, \theta) \subset M$, large n, large d
- $\alpha = \frac{\tan^2\left(\sqrt{\kappa\theta^2}\right)}{\kappa\theta^2}$




Convergence rate modulation factor, sphere dim=3, n=2
Small variance prediction
Asymptotic prediction
Measured
Modulation factor α
Standard deviation θ
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1
2
3
4
5
6
7
8
9


Convergence rate modulation factor, sphere, dim=3, N > 5
Small variance prediction
Asymptotic prediction
N=10
N=20
N=50
N=100
Modulation factor α
Standard deviation θ
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0.6
0.8
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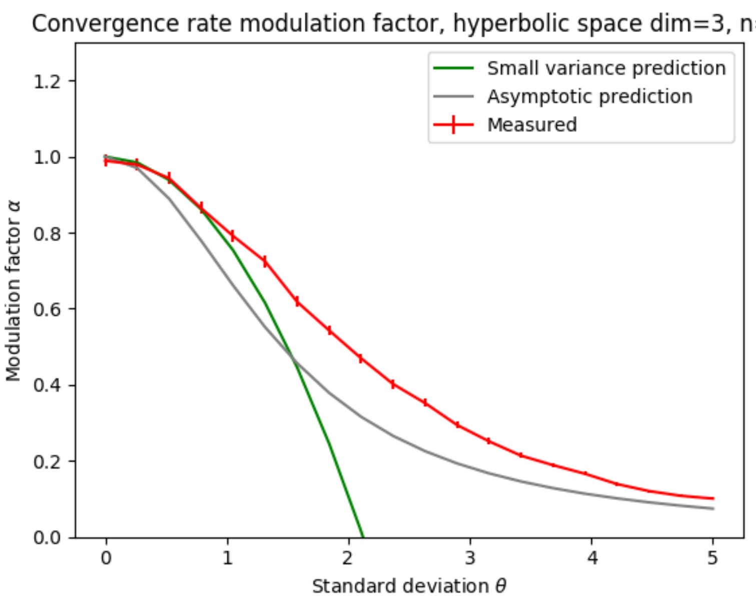
1.2
1.4
1.6
2
4
6
8
10
12


Convergence rate modulation factor, hyperbolic space dim=3, n=2
Small variance prediction
Asymptotic prediction
Measured
Modulation factor α
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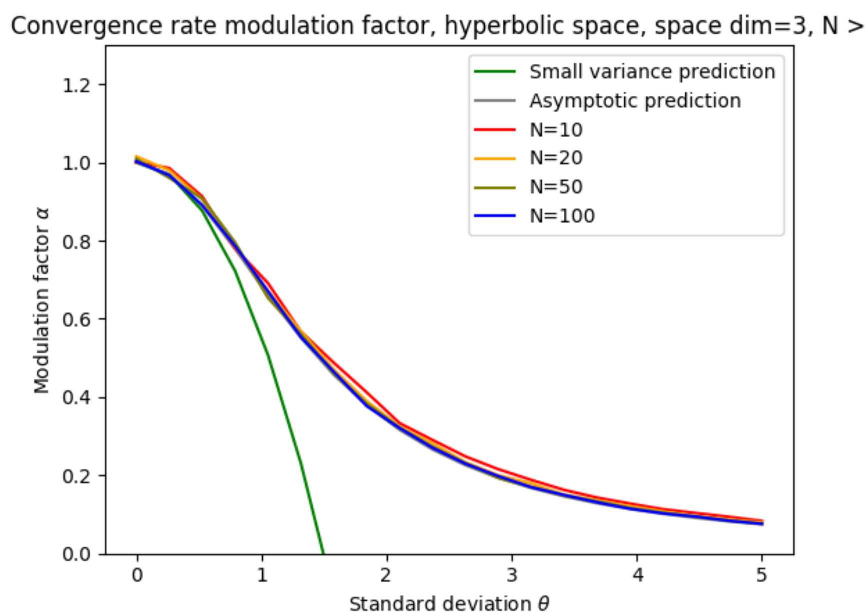
0.6
0.8
1.0
1.2


Convergence rate modulation factor, hyperbolic space, space dim=3, N > 5
Small variance prediction
Asymptotic prediction
N=10
N=20
N=50
N=100
Modulation factor α
Standard deviation θ
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1
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3
4
5
0.0
0.2
0.4
0.6
0.8
1.0
1.2

Conclusions

High concertation expansion very accurate for low theta

Asymptotic expansion very accurate for n> 10

Main variable controlling the modulation is variance-curvature tensor

$$R(\blacksquare, {}^{\circ})\blacksquare : \mathfrak{M}_2$$

Main variable controling the bias

$$\mathfrak{M}_2 : \nabla \circ R({}^{\circ}, \blacksquare)\blacksquare : \mathfrak{M}_2$$

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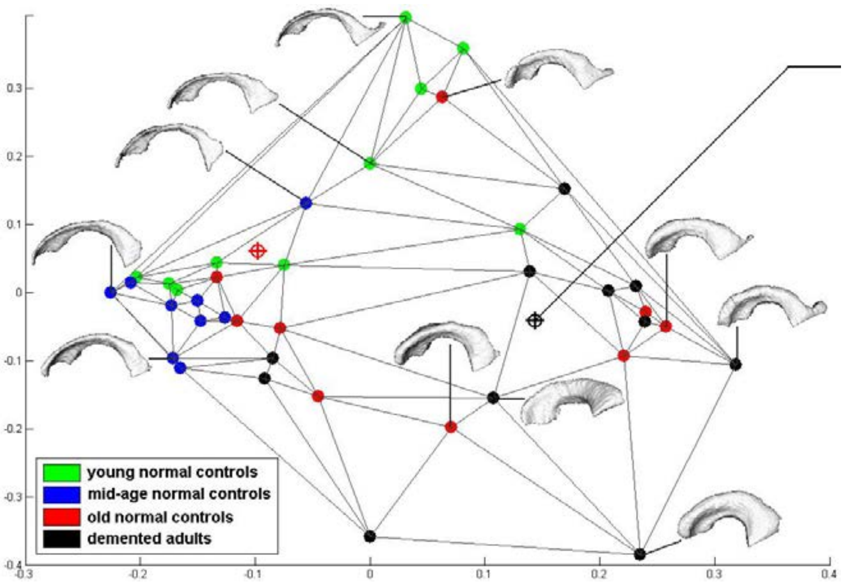
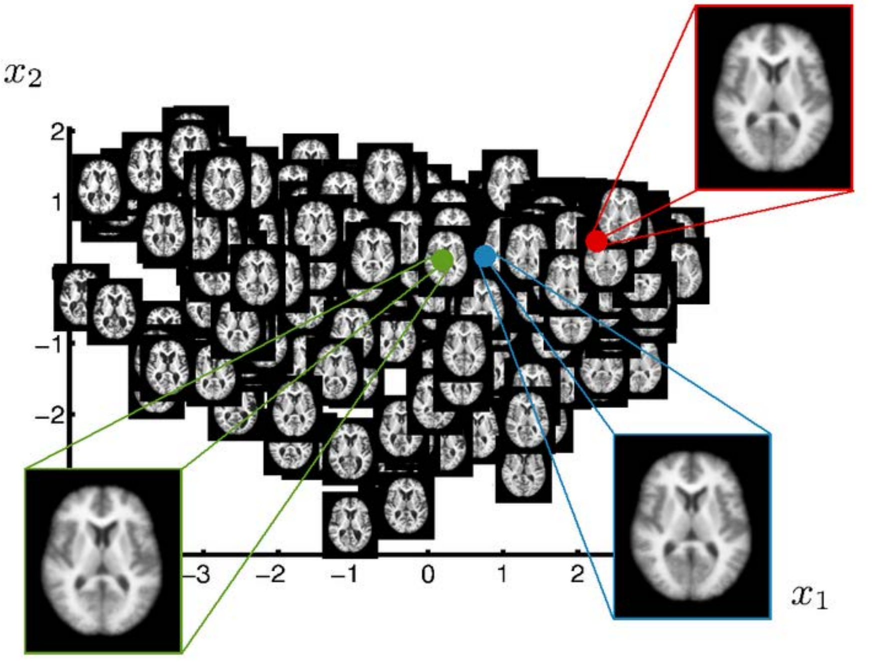
Low dimensional subspace approximation?



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?**

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 $\Sigma(x) \propto \sum_i \overrightarrow{\bar{x}x_i}\,\overrightarrow{\bar{x}x_i}^t$

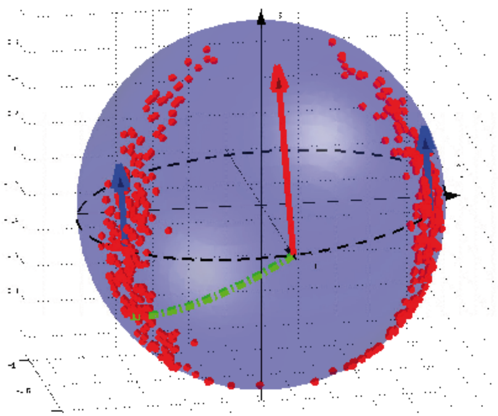
- Generative model:
  - Gaussian (large variance) in the horizontal subspace
  - Gaussian (small variance) in the vertical space

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

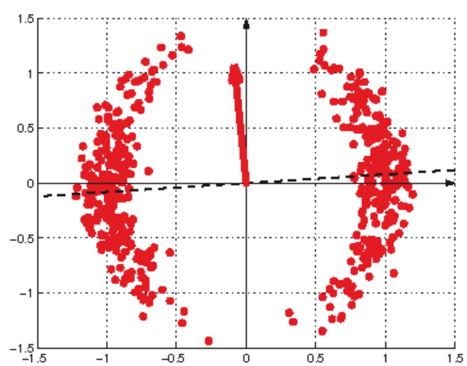
Problems of tPCA

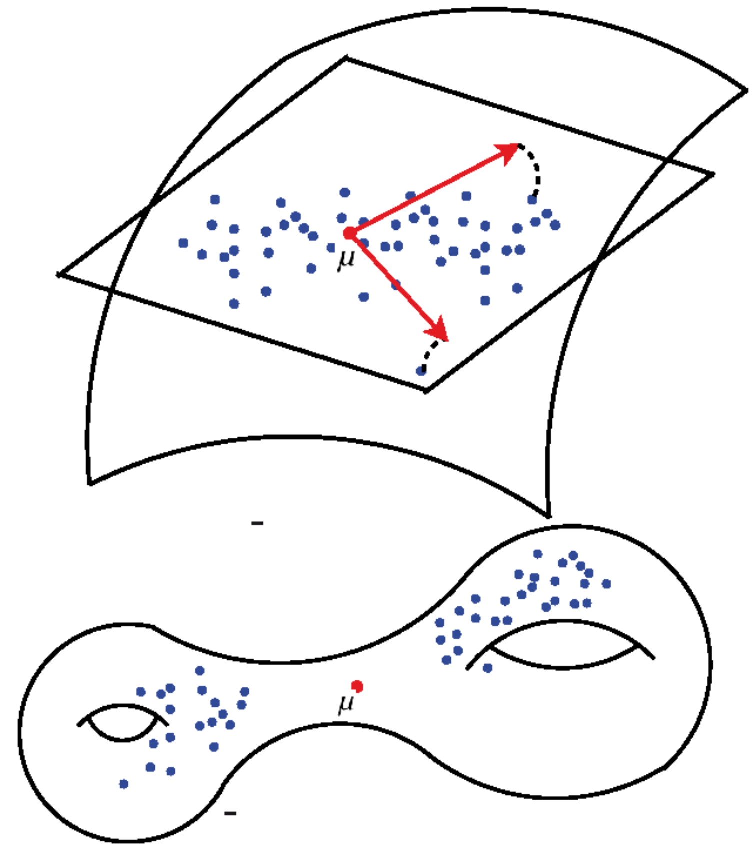
Analysis is done relative to the mean

- 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

Patching the Problems of tPCA / PGA

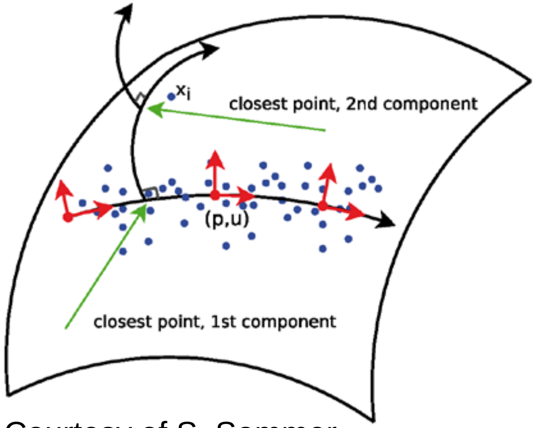
Improve the flexibity of the geodesics

- 1D regression with higher order splines **[Gu, Machado, Leite, Vialard, Singh, Niethammer, Absil,…]**
  - **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**

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Affine span in Euclidean spaces

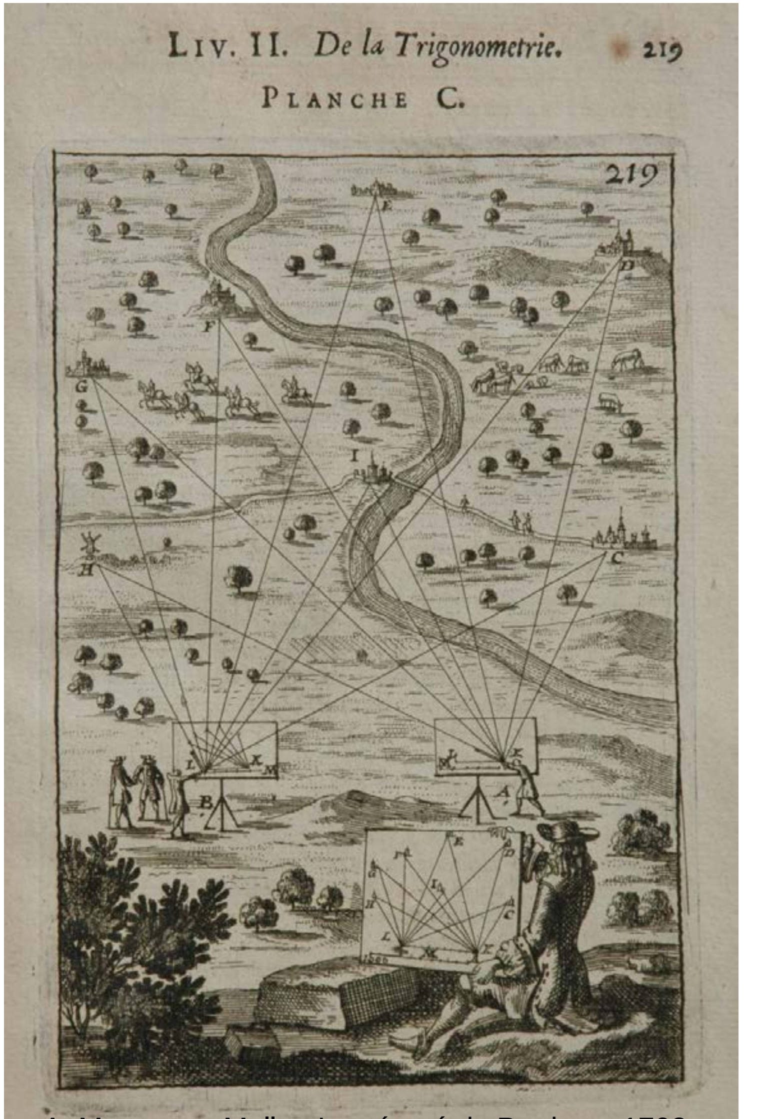
Affine span of (k+1) points: weighted barycentric equation

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

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)

- 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 λ-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 $\quad Aff(x_0, \dots x_k) = \overline{EBS(x_0, \dots x_k)}$

Questions

- Local structure: local manifold? dimension? stratification?
- Relationship between KBS ⊂ FBS, EBS and affine span?

[X.P. Barycentric Subspace Analysis on Manifolds. Annals of statistics. 2018. arXiv:1607.02833]

Analysis of Barycentric Subspaces

Assumptions:

- Restrict to the **punctured manifold** $M^*(x_0, \dots x_k) = M \,/ \cup C(x_i)$
  - $dist^2(x, x_i)$, $\log_x(x_i)$ are smooth but M^* may be split in pieces
- Affinely independent points:
  $\{\overrightarrow{x_i x_j}\}_{0 \le i \neq j \le k}$ exist and are linearly independent 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: $Z(x) = [\,\overrightarrow{x x_0}, \dots \overrightarrow{x x_k}] = U(x)S(x)V^t(x)$
  - $EBS(x_0, \dots x_k) =$ Zero level-set of l>0 singular values of Z(x)
  - Stratification on the number of vanishing singular values

[X.P. Barycentric Subspace Analysis on Manifolds. Annals of statistics. 2018. arXiv:1607.02833]

Analysis of Barycentric Subspaces

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

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

Caractérisation of local minima: Hessian (if non degenerate)

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

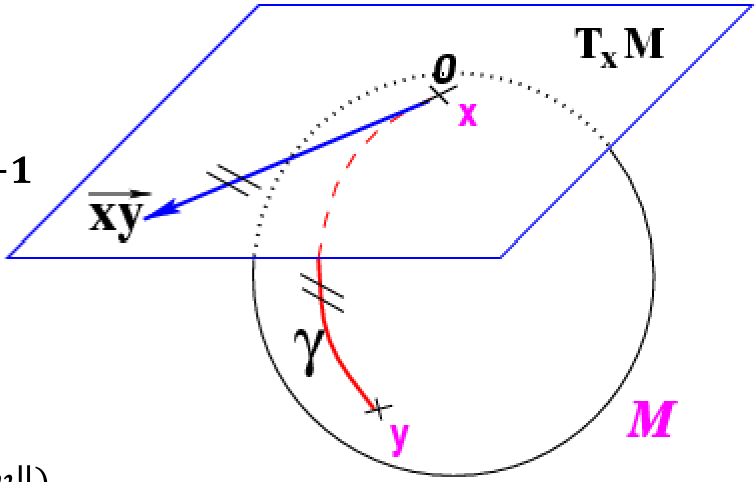
Regular and positive pts (non-degenerated critical points)

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

Theorem: EBS partitioned into cells by the index of the Hessian of λ-variance: KBS = EBS^+ on M*

[X.P. Barycentric Subspace Analysis on Manifolds. Annals of statistics. 2018. arXiv:1607.02833]

Example on the sphere



Manifold

- Unit sphere $\mathcal{M} = \boldsymbol{S_n}$ embedded in $\mathbb{R}^{n+1}$
- ||x|| =1

Exp and log map

$$\exp_x(v) = \cos(\|v\|)\, x + \frac{\sin(\|v\|)}{\|v\|} v$$

$$\log_x(y) = f(\theta)(y - \cos(\theta)) \quad \text{with} \quad \theta = \arccos(x^t y)$$

Distance

$$dist(x, y) = \|\log_x(y)\| = \theta$$

(k+1)-pointed & punctured Sphere

- $X = [x_0, x_1, \dots, x_k] \in (S_n)^k$
- Punctured sphere: exclude antipodal points: $S_n^* = S_n / -X$

KBS / FBS with 3 points on the sphere

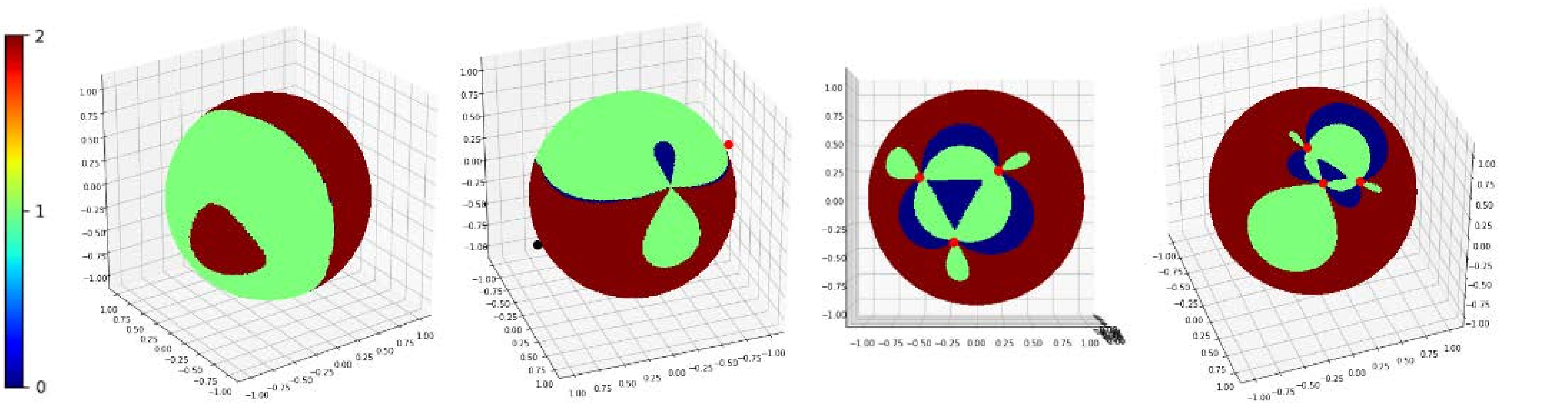
EBS: great subspheres spanned by reference points (mod cut loci)

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

KBS/FBS: look at index of the Hessian of λ-variance

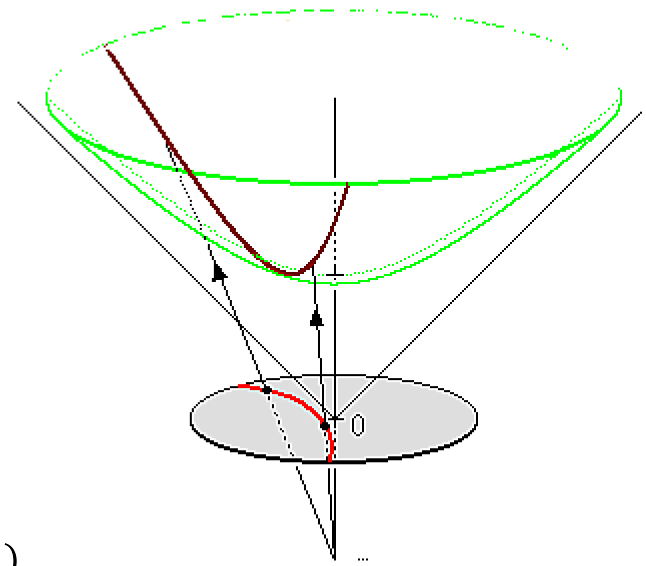
$$\mathrm{H}(\mathrm{x},\lambda) = \sum \lambda_i \theta_i \cot(\theta_i)\,(\mathrm{Id} - \mathrm{xx}^{\mathrm{t}}) + \sum (1 - \lambda_i \theta_i \cot(\theta_i))\, \overrightarrow{x x_i}\, \overrightarrow{x x_i}^{t}$$

- Complex algebric geometry problem [Buss & Fillmore, ACM TG 2001]
- 3 points of the n-sphere: EBS partitioned in cell complex by index of critical point
- **KBS/EBS less interesting than EBS/affine span**



Weighed Hessian index: **brown = -2 (min) = KBS** / green = -1 (saddle) / blue = 0 (max)

Example on the hyperbolic space



Manifold

- Unit pseudo-sphere $\mathcal{M} = \boldsymbol{H_n}$ embedded in Minkowski space $\mathbb{R}^{\mathbf{1},\boldsymbol{n}}$
- $\|x\|_*^2 = -x_0^2 + x_1^2 + \cdots x_n^2 = -1$

Exp and log map

$$\exp_x(v) = \cosh(\|v\|_*)\, x + \frac{\sinh(\|v\|_*)}{\|v\|_*} v$$

$$\log_x(y) = f_*(\theta)(y - \cosh(\theta)) \quad \text{with} \quad \theta = \mathrm{arcosh}(-\langle x|y\rangle_*)$$

Distance $dist(x, y) = \|\log_x(y)\|_* = \theta$

Punctured hyperbolic space: no cut locus to exclude

Example on the hyperbolic space

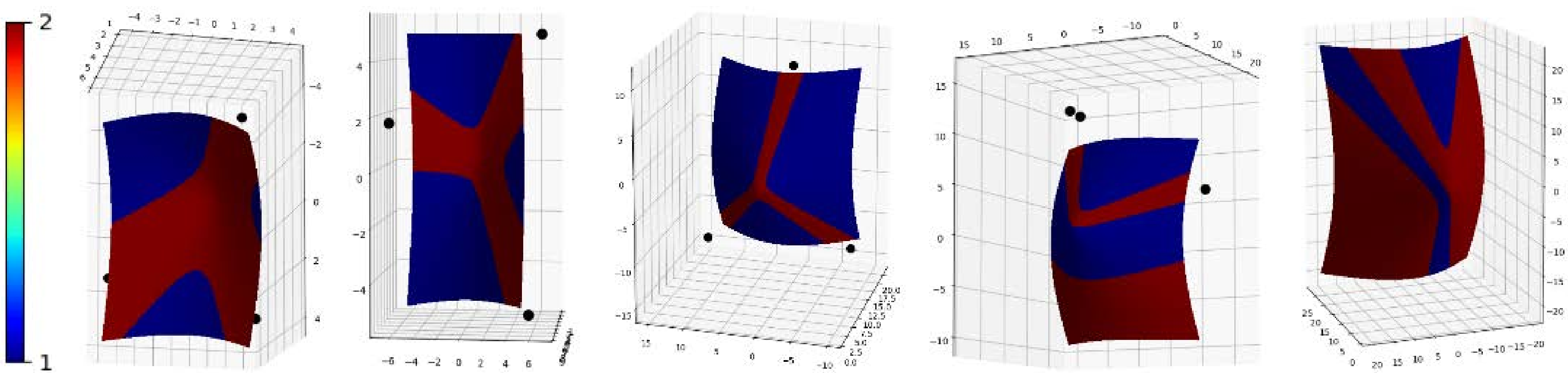
EBS = Affine span: great sub-hyperboloids spanned by reference points

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

KBS: locus of maximal index of the Hessian of λ-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
- 3 points on H^n: better than for spheres, but still disconnected components



Weighted Hessian Index: **brown = -2 (min) = KBS** / blue = 1 (saddle)

Geodesic subspaces are limit cases of affine span

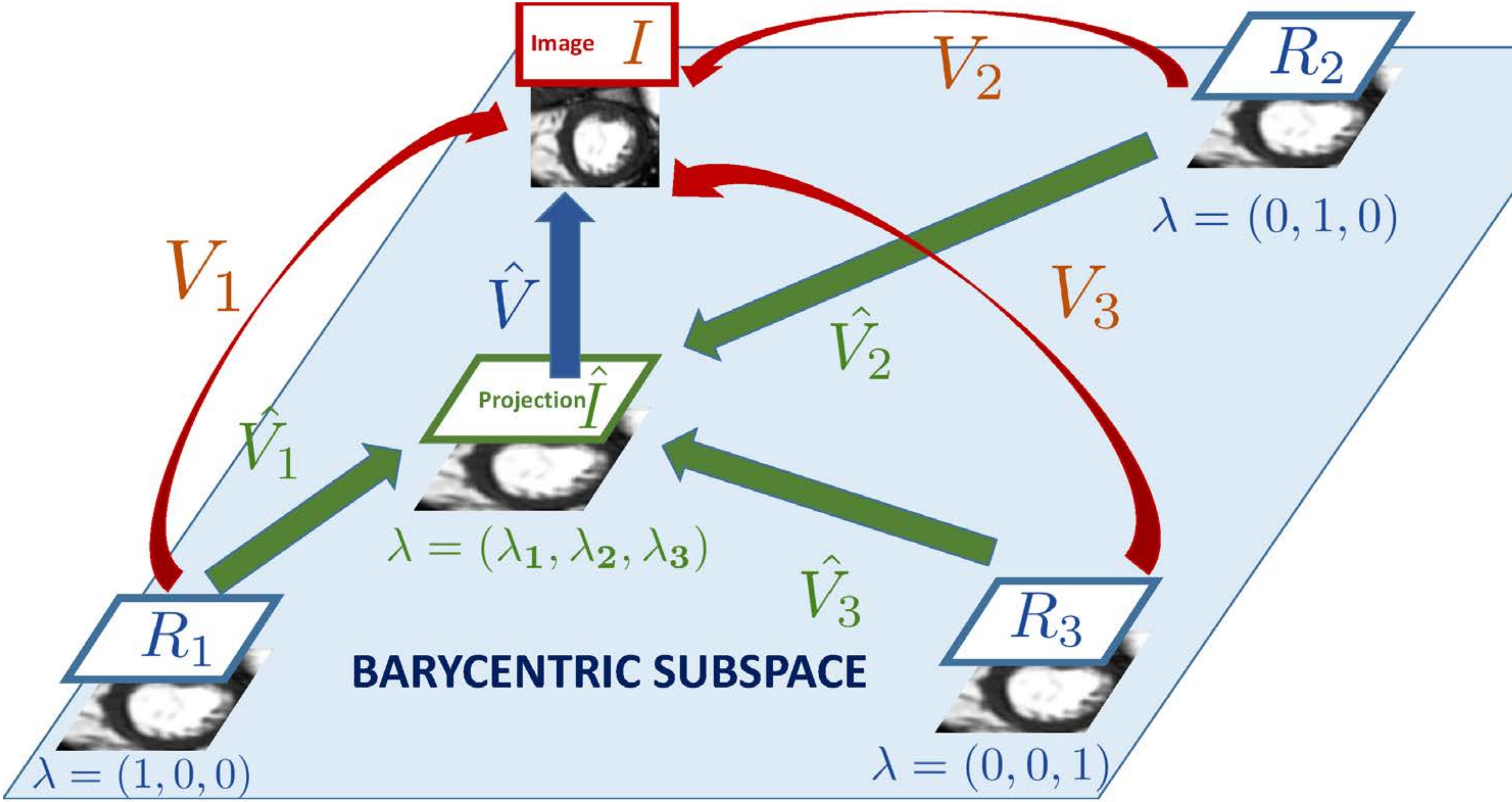
Theorem

- $GS(x, w_1, \dots w_k) = \{\exp_x(\sum_i \alpha_i w_i) \; for \; \alpha \in R^k \}$ is the limit of $Aff\left(x_0, \exp_{x_o}(\epsilon\, w_1), \dots \exp_{x_o}(\epsilon\, w_k)\right)$ when $\epsilon \to 0$.
- Reference points converge to a 1st order (k,n)-jet
  - PGA [Fletcher et al. 2004, Sommer et al. 2014]
  - GPGA [Huckemann et al. 2010]

Conjecture

- This can be generalized to higher order derivatives
  - Quadratic, cubic splines [Vialard, Singh, Niethammer]
  - Principle nested spheres [Jung, Dryden, Marron 2012]
  - Quotient of Lie group action [Huckemann, Hotz, Munk, 2010]

Application in Cardiac motion analysis

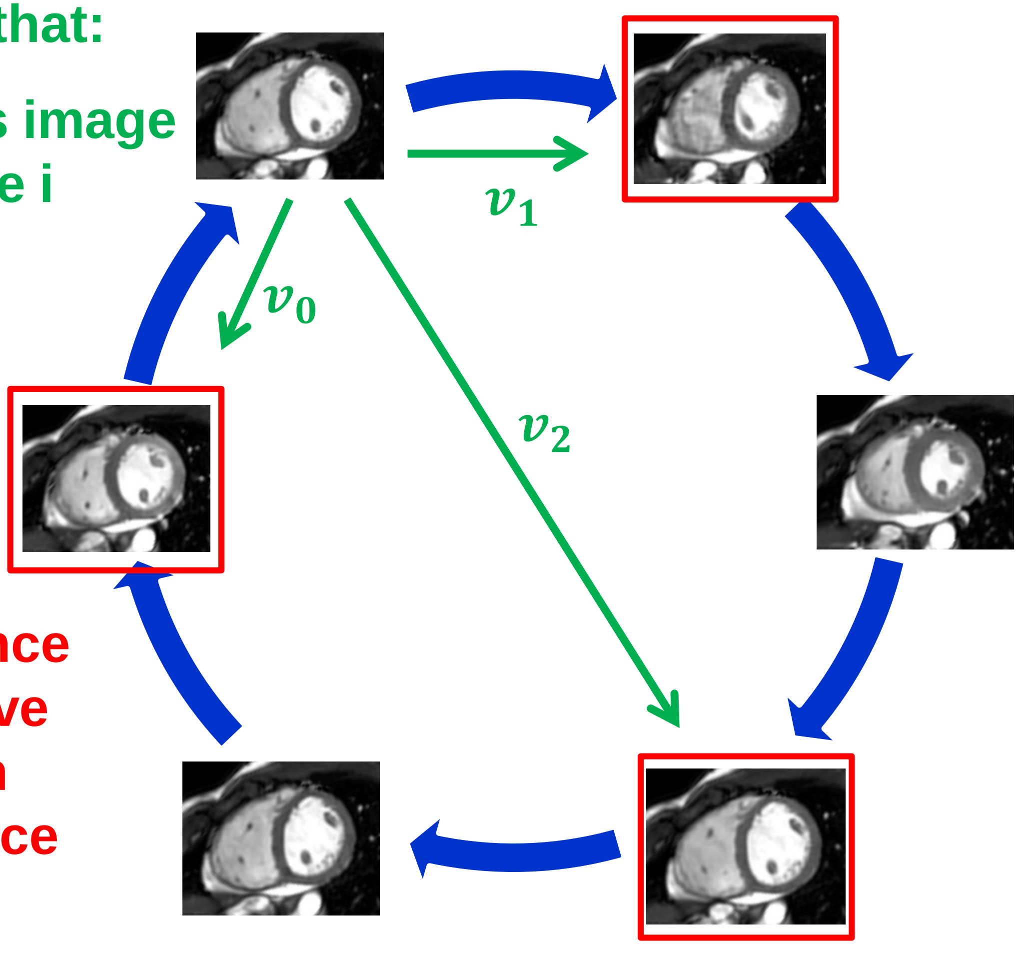


[Marc-Michel Rohé et al., MICCAI 2016, MedIA 45:1-12, 2018]

Application in Cardiac motion analysis

Find weights λ_i and SVFs v_i such that:

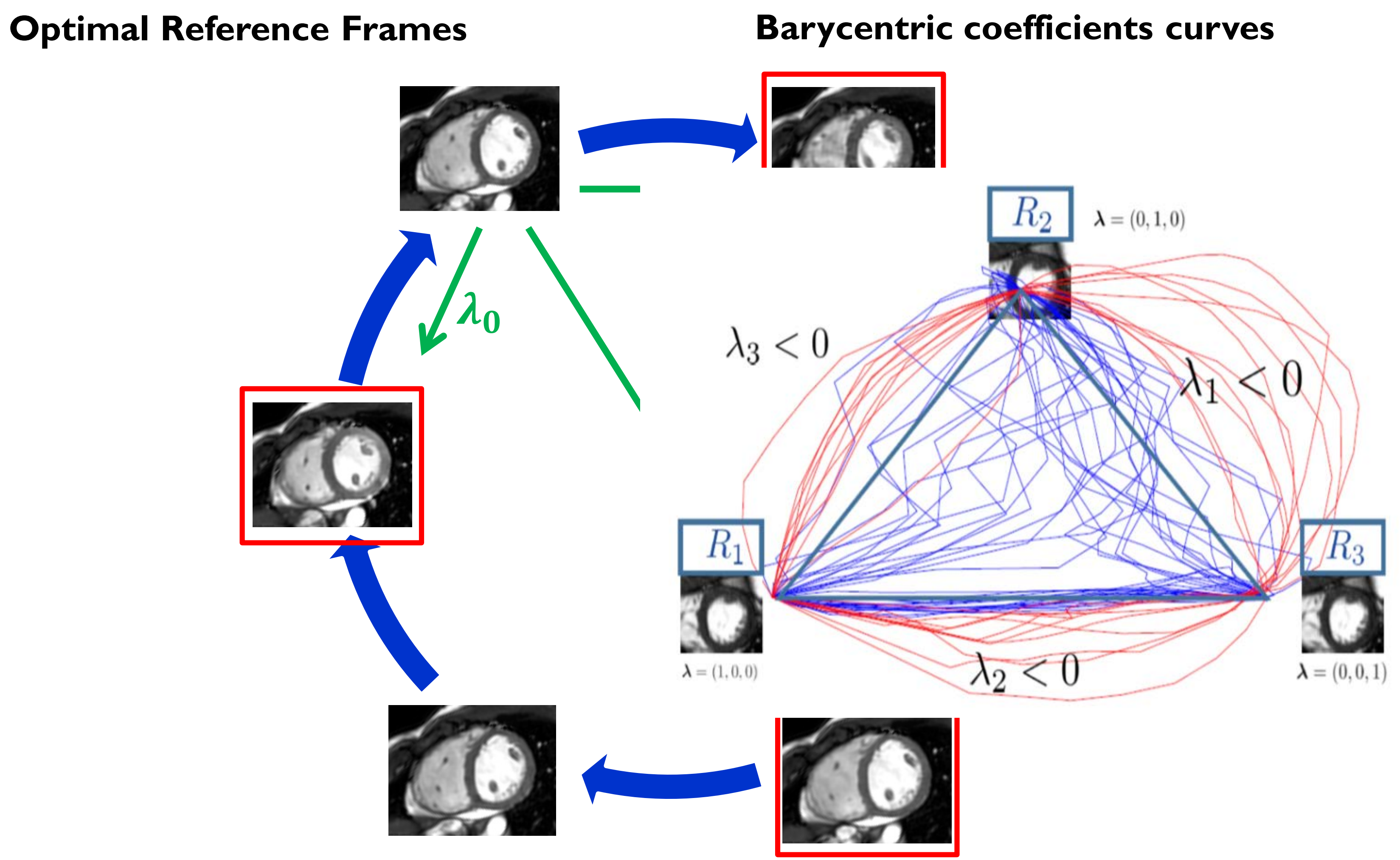
- v_i **registers image to reference i**
- $\sum_i \lambda_i v_i = 0$



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

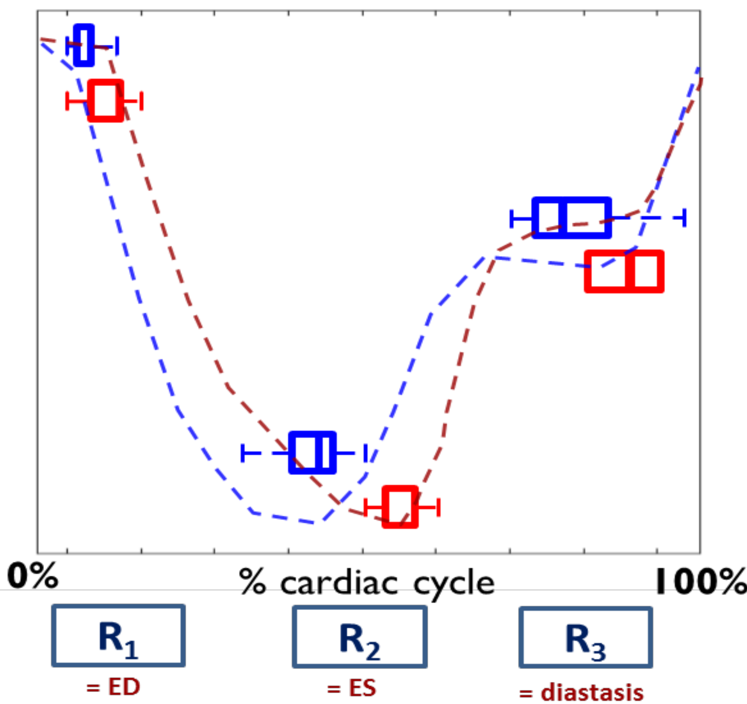


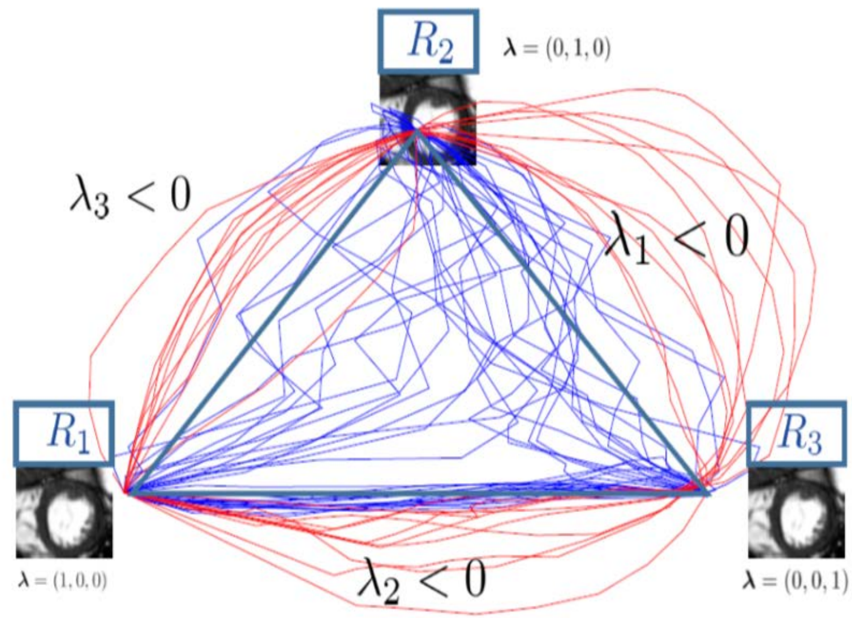
[Marc-Michel Rohé et al., MICCAI 2016, MedIA 45:1-12, 2018]

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**

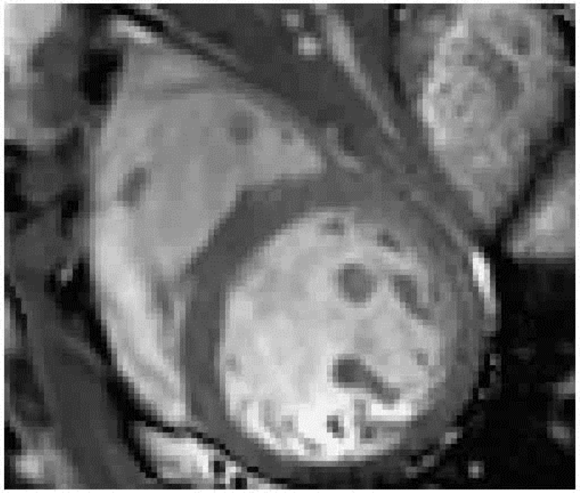
Tested on **10 controls** [1] and **16 Tetralogy of Fallot** patients [2]

[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)

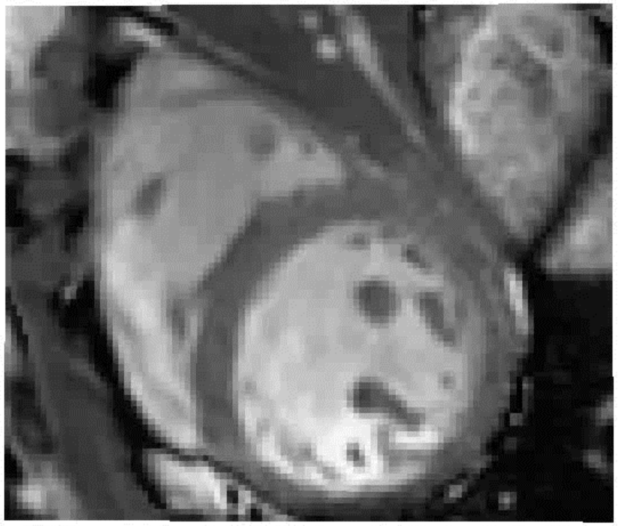
Cardiac motion synthesis

Original Sequence



30 images

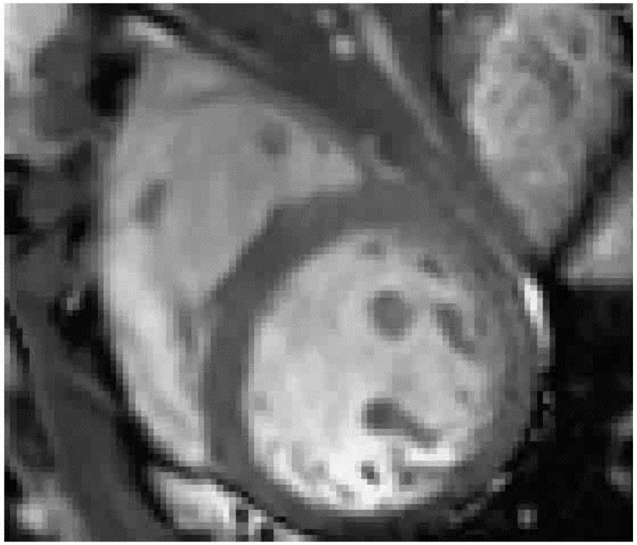
Barycentric Reconstruction (3 images)



3 images + 2 coeff.

Reconstr. error: 18.75
Compression ratio: 1/10

PCA Reconstruction (2 modes)



1 image + 2 SVF + 2 coeff.

Reconstr. error: 26.32 (+40%)
Compression ratio: 1/4

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

Geometric Statistics: Mathematical foundations and applications in computational anatomy

Intrinsic Statistics on Riemannian Manifolds

Manifold-Valued Image Processing

Metric and Affine Geometric Settings for Lie Groups

Parallel Transport to Analyze Longitudinal Deformations

Advances Statistics: CLT & PCA

- Estimation of the empirical Fréchet mean & CLT
- Principal component analysis in manifolds
- Natural subspaces in manifolds: barycentric subspaces
- Rephrasing PCA with flags of subspaces

Forward, Backward and Nested Analysis

Forward Barycentric Subspace (k-FBS) decomposition

- Iteratively add points x_j from j=0 to k
- $x_0 = Mean(y_j), \quad x_1 = argmin_x(\sigma^2_{out}(x_0, x)) \dots$ PGA-like
- Start with 2 points: $(x_0, x_1) = \mathrm{argmin}_{(x,y)}(\sigma^2_{out}(x, y))$ GPGA-like

Backward analysis: Pure Barycentric Subspace (k-PBS)

- Find $Aff(x_0, \dots x_k)$ minimizing the unexplained variance:

$$\sigma^2_{out}(x_0, \dots x_k) = \sum_j dist^2\left(y_j, Proj_{Aff(x_0 \dots x_k)}(y_j)\right)$$

- Iteratively remove one point from $(x_0, \dots x_j)$ from j=0 to k
- One optimization only for k+1 points and discrete backward reordering

From greedy to global optimization?

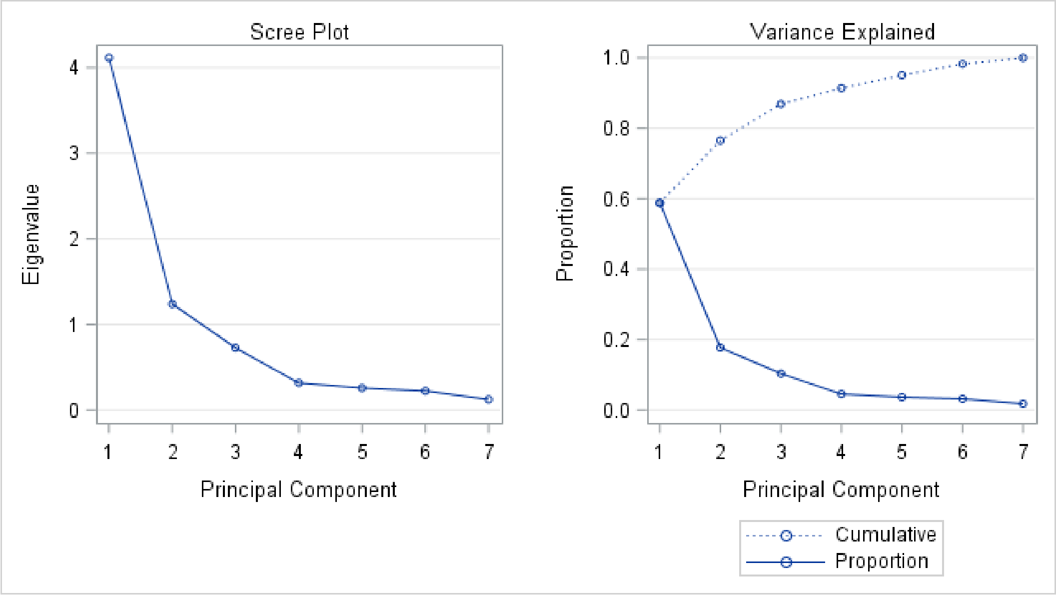
- Optimal unexplained variance → non nested subspaces
- Nested forward / backward procedures → not optimal
- Optimize first, decide dimension later → Nestedness required
  [Principal nested relations: Damon, Marron, JMIV 2014]

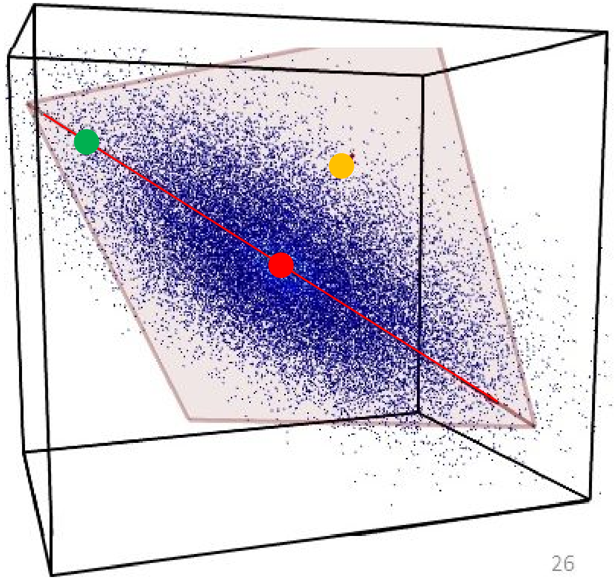
Barycentric Subspace Analysis (k-BSA)

The natural object for PCA: Flags of subspaces in manifolds

- $x_0 \prec x_1 \prec \cdots \prec x_k$ are k +1 n distinct ordered points of M.
- $FL(x_0 \prec x_1 \prec \cdots \prec x_k)$ is the sequence of properly nested subspaces $FL_{i(x_0 \prec x_1 \prec \cdots \prec x_k)} = Aff(x_0, \ldots x_i)$

$$Aff(x_0) = \{x_0\} \subset \ldots Aff(x_0, \ldots x_k) \ldots \subset Aff(x_0, \ldots x_n) = M$$
$$\sigma^2_{out}(x_0) \geq \ldots \geq \sigma^2_{out}(x_0, \ldots x_k) \geq \ldots \geq \sigma^2_{out}(x_0, \ldots x_n) = 0$$





Adapted from 3DM slides by Marc van Kreveld

Barycentric Subspace Analysis (k-BSA)

Accumulated unexplained variance (area under the curve)

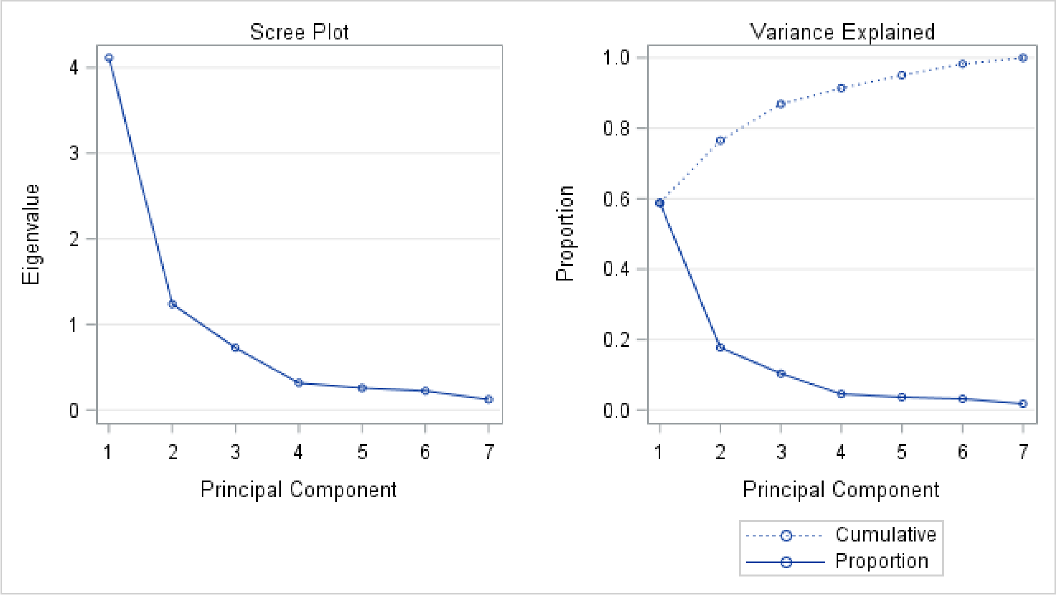
- k-BSA optimizes: $AUV(k) = \sum_{i=0}^{k} \sigma_{out}^2(x_0, \ldots x_i)$
- In a Euclidean space with Gaussian $N(x_0, \Sigma = diag(\sigma_1^2, \ldots \sigma_n^2))$

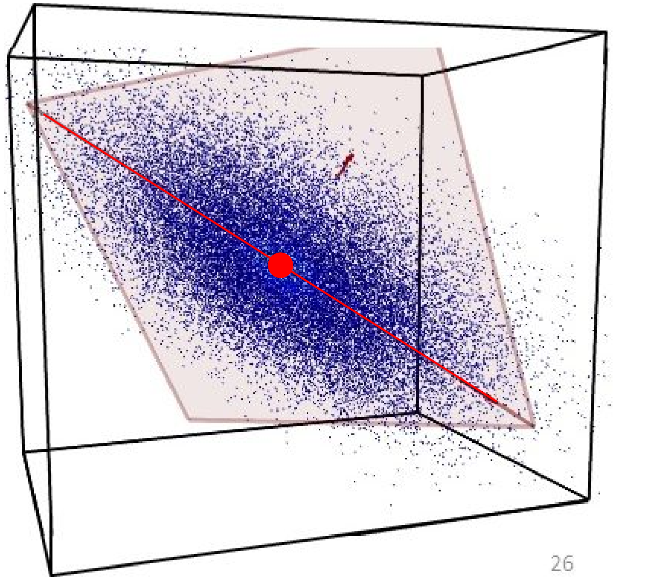
$\sigma_{out}^2(x_0, \ldots x_i) = \sigma_{i+1}^2 + \cdots \sigma_n^2 \rightarrow AUV(k) = \sum_{i=0}^{k} i\, \sigma_i^2 + (k+1) \sum_{i=k+1}^{n} \sigma_i^2$

→ minimal for ordered eigenmodes of Σ with $\sigma_1 \geq \sigma_2 \; \ldots \geq \sigma_n$

\

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



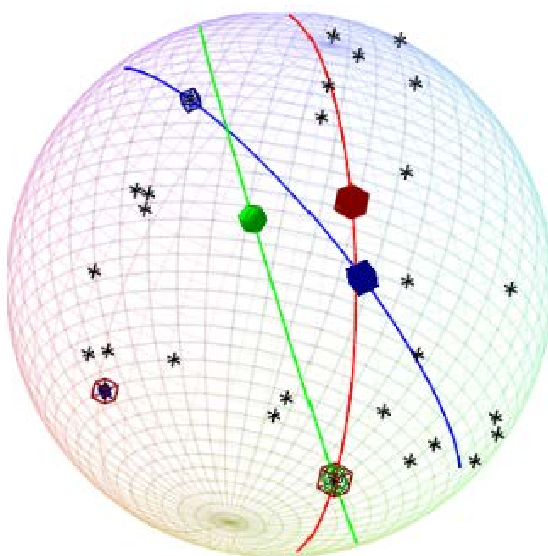


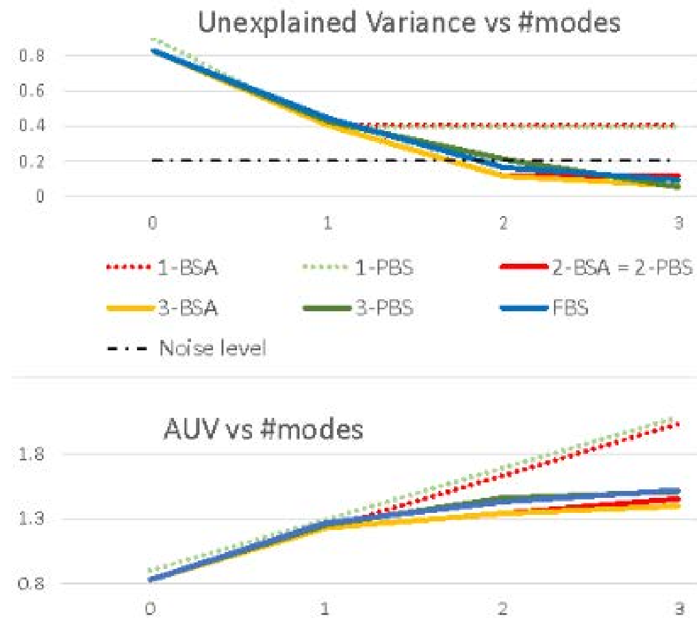
Adapted from 3DM slides by Marc van Kreveld

Sample-limited barycentric subspace inference

Restrict the inference to data points only

- Fréchet mean / template [Lepore et al 2008]
- 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**

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)

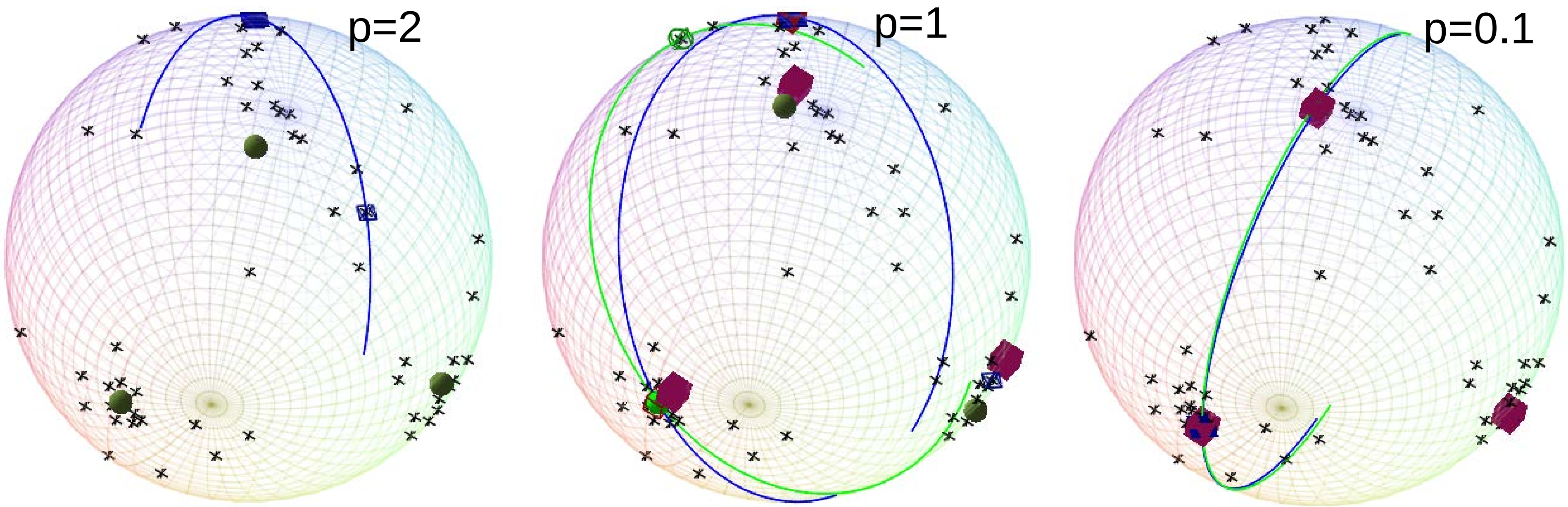
Unexplained p-variance of residuals

- $2 < p \rightarrow +\infty$: 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

Experiments on the sphere

3 clusters on a 5D sphere

- 10, 9 and 8 points (stddev 6 deg) around three orthogonal axes plus 30 points uniformly samples on 5D sphere

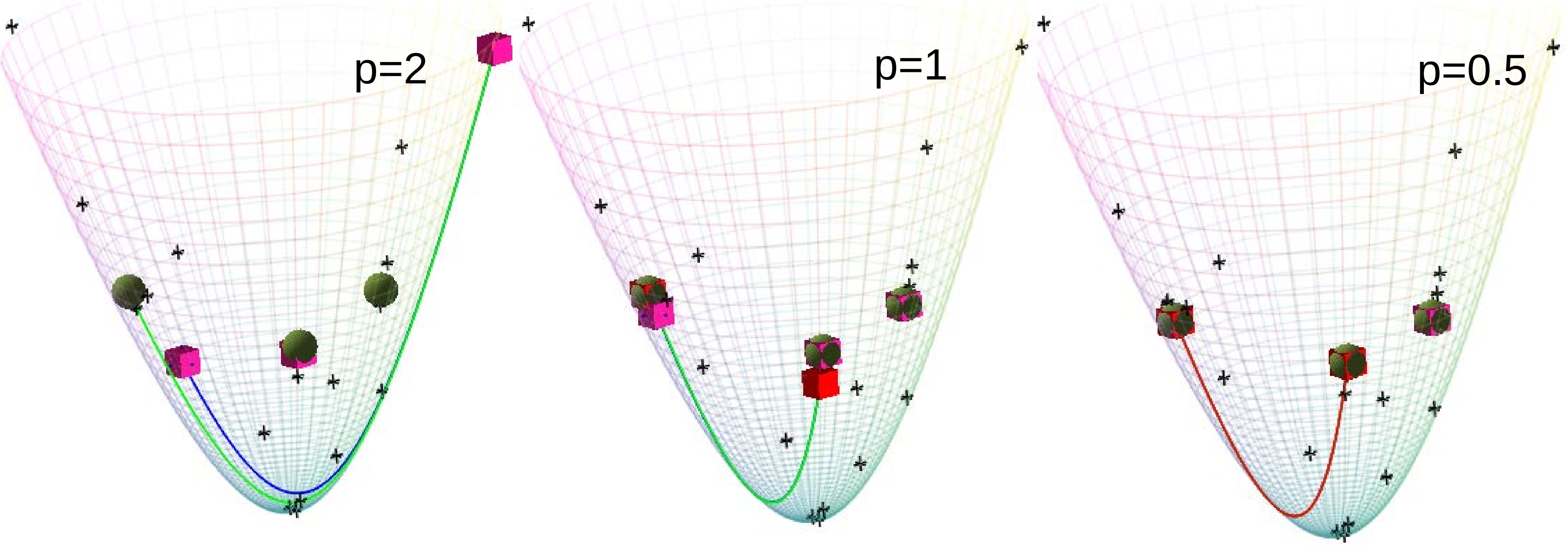


- **FBS: Forward Barycentric Subspace: mean and median not in clusters**
- **1-PBS / 2-PBS: Pure Barycentric Subspace with backward ordering: ok for k=2 only**
- **1-BSA / 2-BSA: Barycentric Subspace Analysis up to order k: less sensitive to p & k**

Experiments on the hyperbolic space

3 clusters on a 5D hyperboloid (50% outliers)

- 15 random points (stddev 0.015) around an equilateral triangle of length 1.57 plus 15 points of stddev 1.0 (truncated at max 1.5)



- **FBS: Forward Barycentric Subspace: ok for $p \leq 0.5$**
- **1-PBS / 2-PBS: Pure Barycentric Subspace with backward ordering: ok for k=2 only**
- **1-BSA / 2-BSA: Barycentric Subspace Analysis up to order k: ok for $p \leq 1$**

Take home messages

Natural subspaces in manifolds

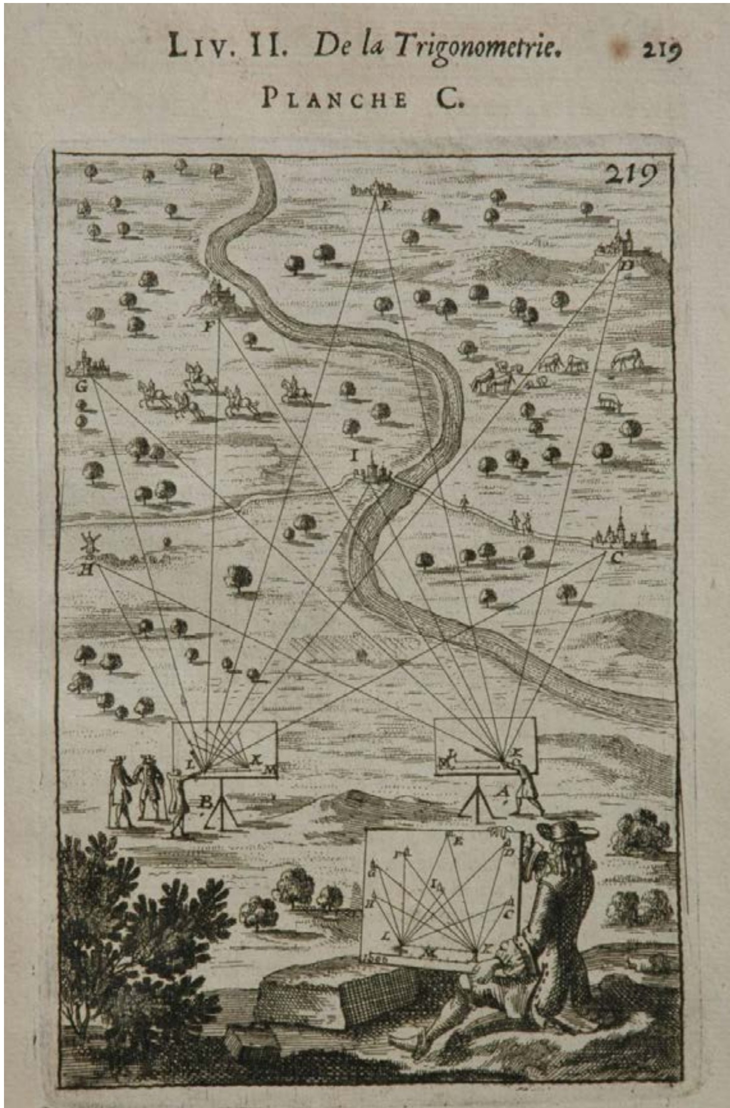
- PGA & Godesic subspaces:
  look at data points from the (unique) mean
- Barycentric subspaces:
  « triangulate » several reference points
  - Justification of multi-atlases?

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

Open research avenues

Other iterative least squares methods?

- ICA, PLS
- Manifold learning → Submanifold learning

Modulate BSA to account for within subspace distribution

- Gaussian: central points
- Clusters: mixtures of modes
- Extremal references: archetypal analysis

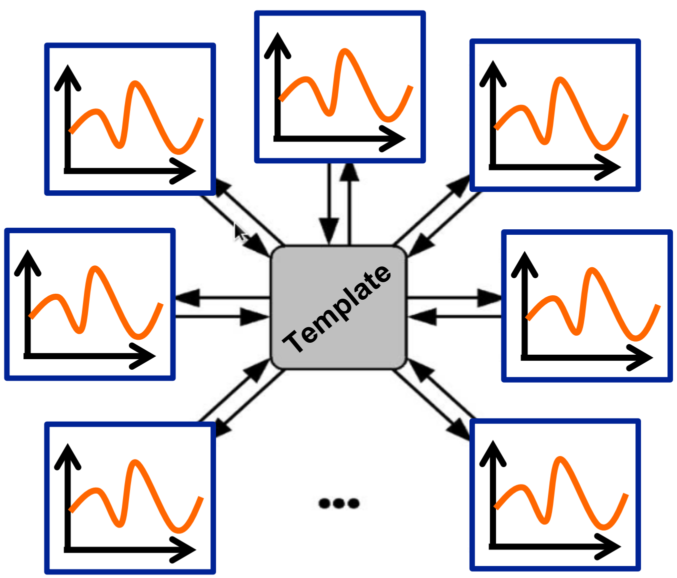
And applications

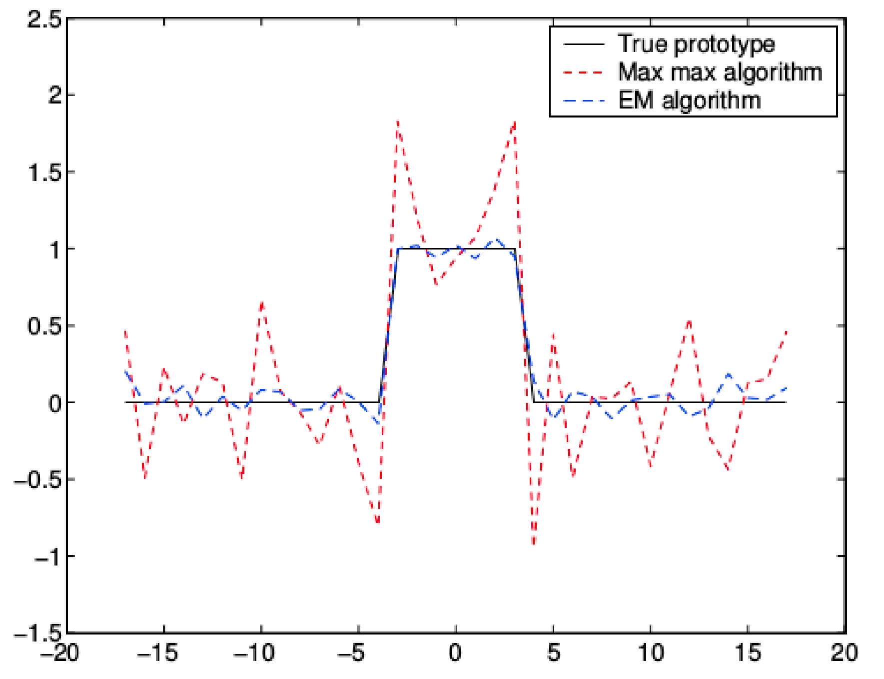
- Multi-atlases (brains, heart motion image sequences)
- SPD matrices (BCI)

Quotient spaces

Functions/Images modulo time/space parameterization

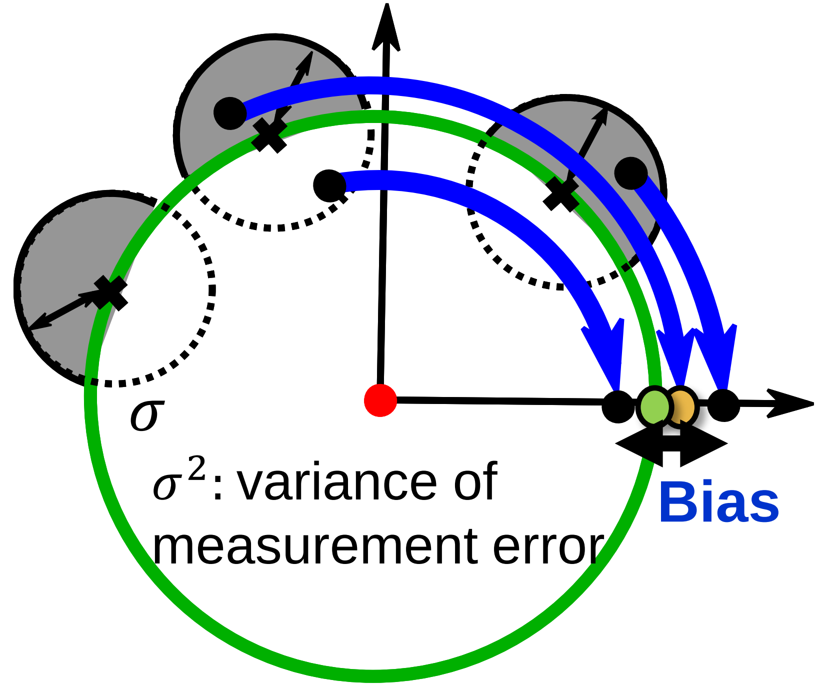
- Amplitude and phase discrimination problem





[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, Allassonnière, Trouvé and XP. SIIMS 2017, Entropy, 2017]

→ Estimated atlas is topologically more complex than should be

References on Barycentric Subpsace Analysis

- **Barycentric Subspace Analysis on Manifolds**
  X. P. Annals of Statistics. 46(6A):2711-2746, 2018. [arXiv:1607.02833]
  - **Barycentric Subspaces and Affine Spans in Manifolds** Geometric Science of Information GSI'2015, Oct 2015, Palaiseau, France. LNCS 9389, pp.12-21, 2015.
    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.
- **Low-Dimensional Representation of Cardiac Motion Using Barycentric Subspaces: a New Group-Wise Paradigm for Estimation, Analysis, and Reconstruction.** M.M Rohé, M. Sermesant and X.P. Medical Image Analysis vol 45, Elsevier, April 2018, 45, pp.1-12.
  - **Barycentric subspace analysis: a new symmetric group-wise paradigm for cardiac motion tracking.** M.M Rohé, M. Sermesant and X.P. Proc of MICCAI 2016, Athens, LNCS 9902, p.300-307, Oct 2016.