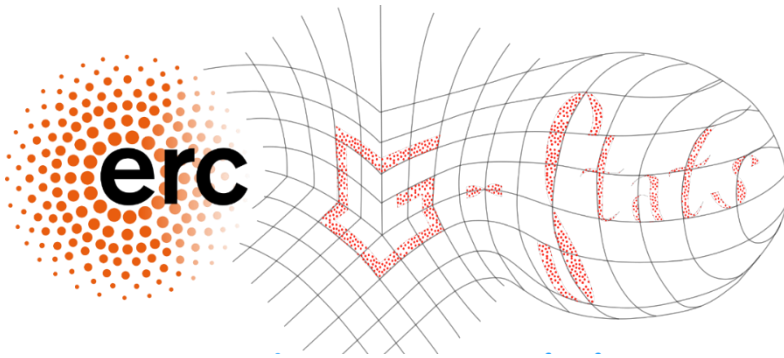


Xavier Pennec

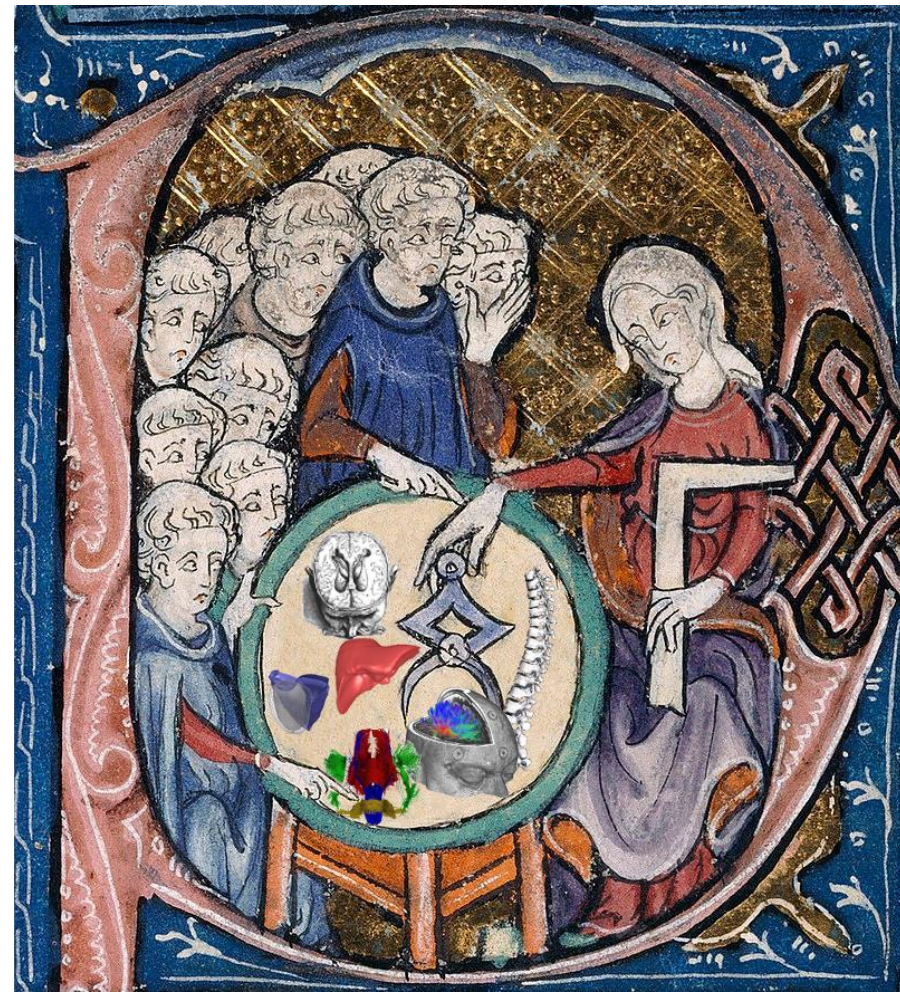
Univ. Côte d'Azur and Inria, France



http://www-sop.inria.fr/asclepios/cours/Peyresq_2019/

Geometric Statistics

*Mathematical foundations
and applications in
computational anatomy*



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

3/ Metric and Affine Geometric Settings for Lie Groups

Ecole d'été de Peyresq, Jul 1-5 2019



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

Geometric Statistics: Mathematical foundations and applications in computational anatomy

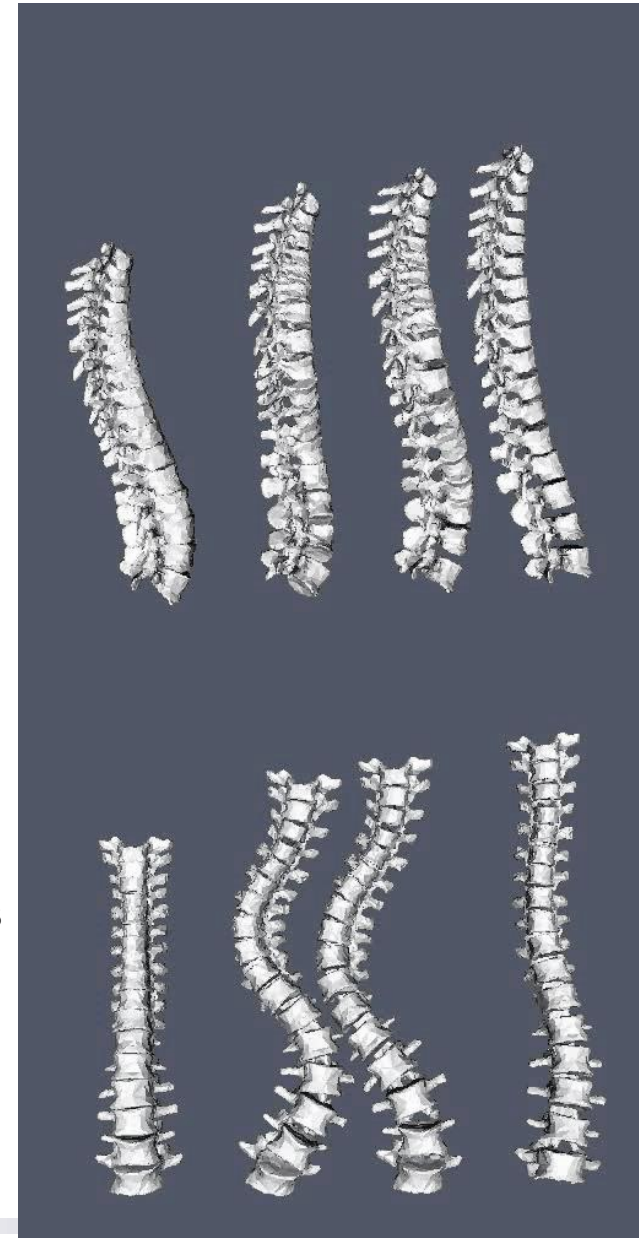
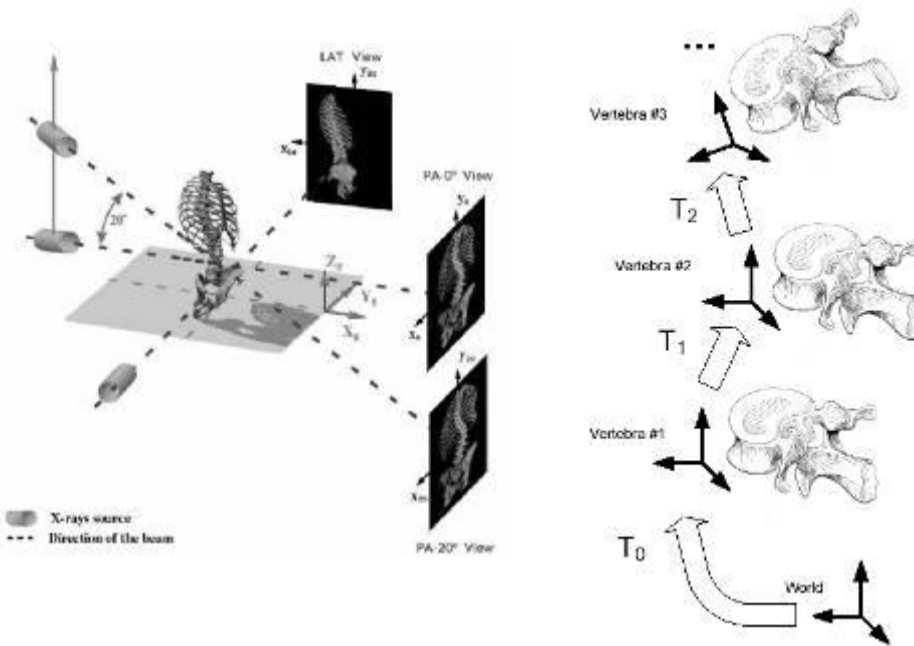
**Intrinsic Statistics on Riemannian Manifolds
Manifold-Valued Image Processing**

Metric and Affine Geometric Settings for Lie Groups

- Riemannian frameworks on Lie groups
- Lie groups as affine connection spaces
- Bi-invariant statistics with Canonical Cartan connection
- The SVF framework for diffeomorphisms

**Parallel transport to analyze Longitudinal deformations
Advances Statistics: CLT & PCA**

Statistical Analysis of the Scoliotic Spine



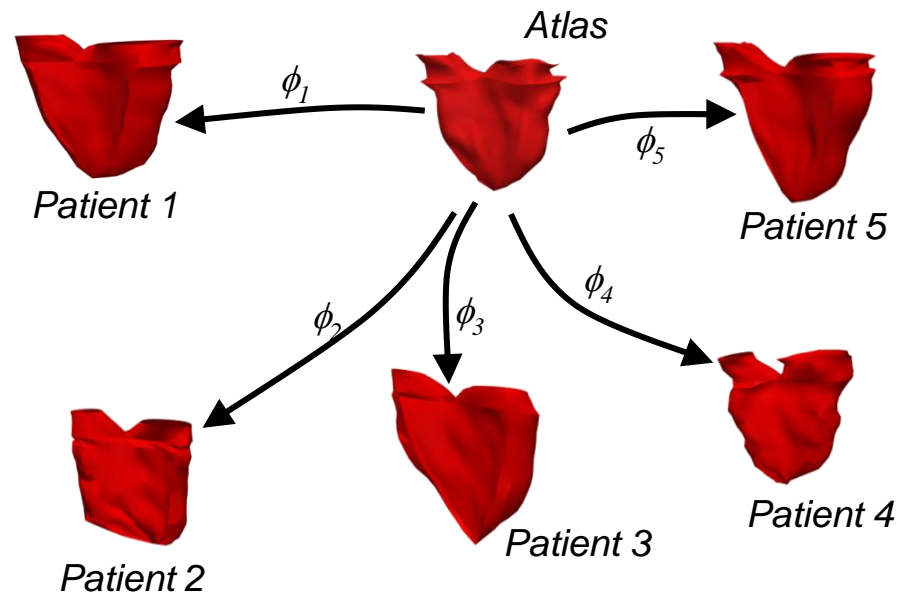
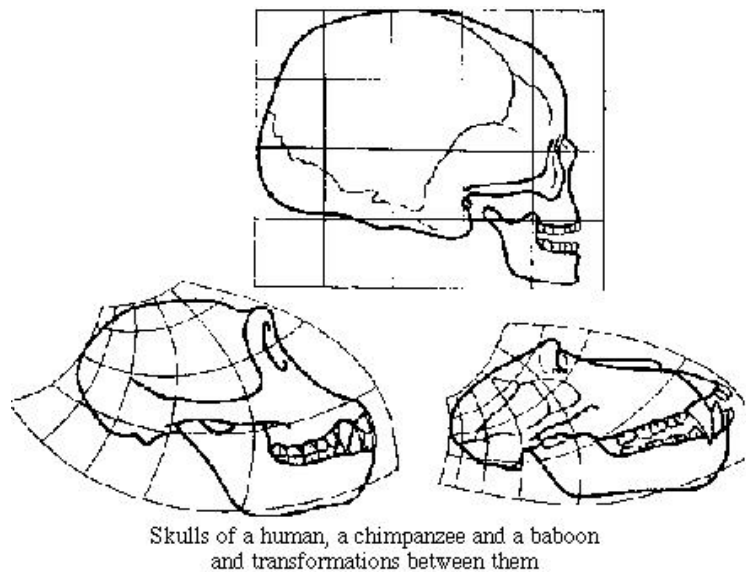
Data

- 307 Scoliotic patients from the Montreal's St-Justine Hosp
- 3D Geometry from multi-planar X-rays
- Articulated model: 17 relative pose of successive vertebrae

Statistics

- Main translation variability is axial (growth?)
- Main rot. var. around anterior-posterior axis
- **4 first variation modes related to King's classes**

Morphometry through Deformations



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

- Observation = “random” deformation of a reference template
- Deterministic template = anatomical invariants [Atlas ~ mean]
- Random deformations = geometrical variability [Covariance matrix]

Natural Riemannian Metrics on Transformations

Transformation are Lie groups: Smooth manifold G compatible with group structure

- Composition $g \circ h$ and inversion g^{-1} are smooth
- Left and Right translation $L_g(f) = g \circ f$ $R_g(f) = f \circ g$
- Conjugation $\text{Conj}_g(f) = g \circ f \circ g^{-1}$

Natural Riemannian metric choices

- Chose a metric at Id: $\langle x, y \rangle_{\text{Id}}$
- Propagate at each point g using left (or right) translation
 $\langle x, y \rangle_g = \langle DL_{g^{(-1)}} \cdot x, DL_{g^{(-1)}} \cdot y \rangle_{\text{Id}}$

Implementation

- Practical computations using left (or right) translations

$$\text{Exp}_f(x) = f \circ \text{Exp}_{\text{Id}}(DL_{f^{(-1)}} \cdot x) \qquad \vec{fg} = \text{Log}_f(g) = DL_f \cdot \text{Log}_{\text{Id}}(f^{(-1)} \circ g)$$

General Non-Compact and Non-Commutative case

No Bi-invariant Mean for 2D Rigid Body Transformations

□ Metric at Identity: $dist(Id, (\theta; t_1; t_2))^2 = \theta^2 + t_1^2 + t_2^2$

□ $T_1 = \left(\frac{\pi}{4}; -\frac{\sqrt{2}}{2}; \frac{\sqrt{2}}{2}\right)$ $T_2 = (0; \sqrt{2}; 0)$ $T_3 = \left(-\frac{\pi}{4}; -\frac{\sqrt{2}}{2}; -\frac{\sqrt{2}}{2}\right)$

□ Left-invariant Fréchet mean: $(0; 0; 0)$

□ Right-invariant Fréchet mean: $\left(0; \frac{\sqrt{2}}{3}; 0\right) \simeq (0; 0.4714; 0)$

Questions for this talk:

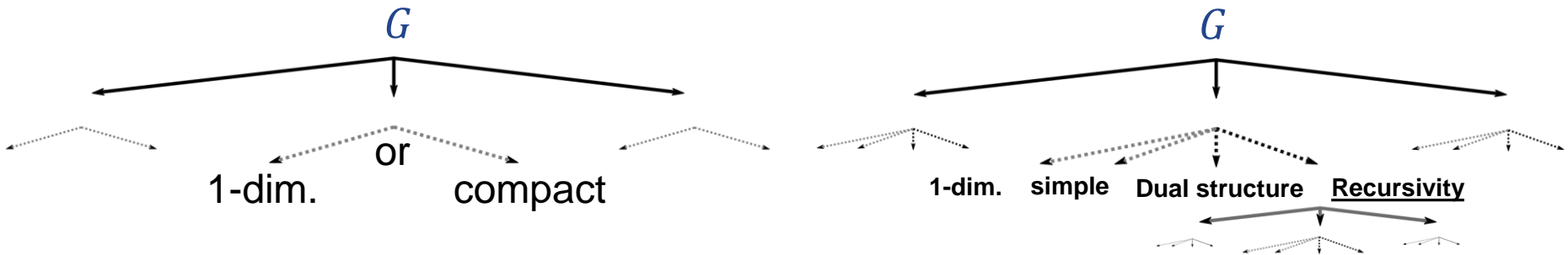
- **Can we design a mean compatible with the group operations?**
- **Is there a more convenient structure for statistics on Lie groups?**

Existence of *bi-invariant (pseudo) metrics*

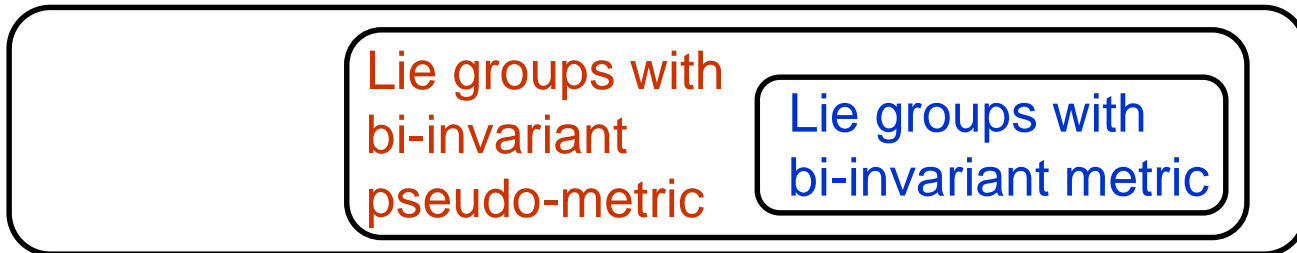
[Cartan 50's]:
Bi-invariant metric on G



[Medina, Revoy 80's]:
Bi-invariant pseudo-metric on G



All
Lie groups



[Miolane, Pennec, Computing Bi-Invariant Pseudo-Metrics on Lie Groups for Consistent Statistics. *Entropy*, 17(4):1850-1881, April 2015.]

- Algorithm: decompose the Lie algebra and find a bi-inv. pseudo-metric
- Test on rigid transformations $SE(n)$: bi-inv. ps-metric for $n=1$ or 3 only

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

- Riemannian frameworks on Lie groups
- **Lie groups as affine connection spaces**
- Bi-invariant statistics with Canonical Cartan connection
- The SVF framework for diffeomorphisms

**Parallel transport to analyze Longitudinal deformations
Advances Statistics: CLT & PCA**

Basics of Lie groups

Flow of a left invariant vector field $\tilde{X} = DL.x$ from identity

- $\gamma_x(t)$ exists for all time
- One parameter subgroup: $\gamma_x(s + t) = \gamma_x(s) \cdot \gamma_x(t)$

Lie group exponential

- Definition: $x \in \mathfrak{g} \rightarrow \text{Exp}(x) = \gamma_x(1) \in G$
- Diffeomorphism from a neighborhood of 0 in \mathfrak{g} to a neighborhood of e in G (not true in general for inf. dim)

3 curves parameterized by the same tangent vector

- Left / Right-invariant geodesics, one-parameter subgroups

Question: Can one-parameter subgroups be geodesics?

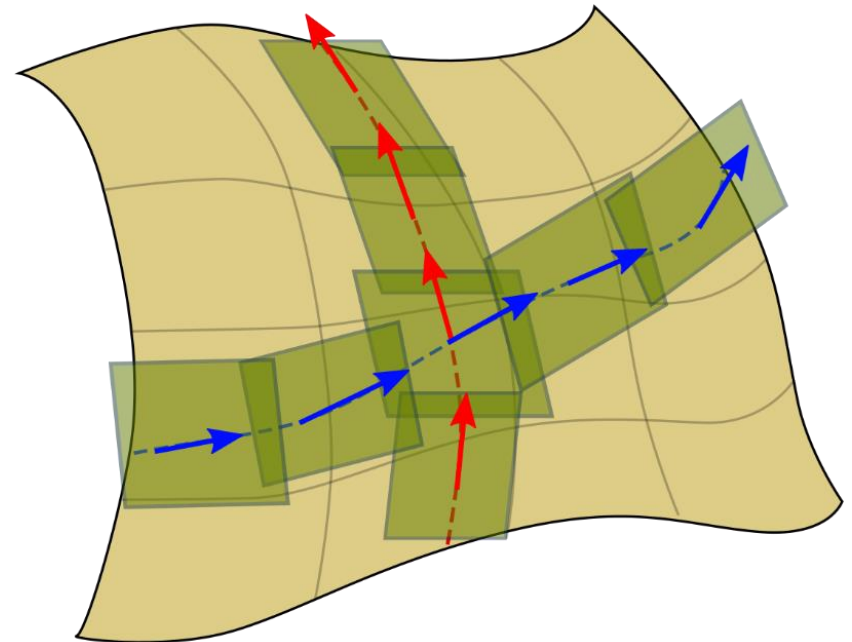
Affine connection spaces: Drop the metric, use connection to define geodesics

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 Affine 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 exist 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: $S_A(M(t)) = A \exp(-tV)A^{-1}A = M(-t)$

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

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

- Riemannian frameworks on Lie groups
- Lie groups as affine connection spaces
- **Bi-invariant statistics with Canonical Cartan connection**
- The SVF framework for diffeomorphisms

**Parallel transport to analyze Longitudinal deformations
Advances Statistics: CLT & PCA**

Mean value on an affine connection space

Fréchet / Karcher means not usable (no distance) but:

$$E[\mathbf{x}] = \operatorname{argmin}_{y \in M} \left(E[\operatorname{dist}(y, \mathbf{x})^2] \right) \Rightarrow E[\overrightarrow{\bar{x}\mathbf{x}}] = \int_M \overrightarrow{\bar{x}\mathbf{x}} \cdot p_{\mathbf{x}}(z) \cdot dM(z) = 0 \quad [P(C) = 0]$$

Exponential barycenters

- [Emery & Mokobodzki 91, Corcuera & Kendall 99]

$$\int \operatorname{Log}_x(y) \mu(dy) = 0 \quad \text{or} \quad \sum_i \operatorname{Log}_x(y_i) = 0$$

- Existence? Uniqueness?
- OK for convex affine manifolds with semi-local convex geometry
[Arnaudon & Li, Ann. Prob. 33-4, 2005]
 - Use a separating function (convex function separating points) instead of a distance
- Algorithm to compute the mean: fixed point iteration (stability?)

Bi-invariant Mean on Lie Groups

Exponential barycenter of the symmetric Cartan connection

- Locus of points where $\sum \text{Log}(m^{-1} \cdot g_i) = 0$ (whenever defined)
- Iterative algorithm: $m_{t+1} = m_t \circ \text{Exp}\left(\frac{1}{n} \sum \text{Log}(m_t^{-1} \cdot g_i)\right)$
- First step corresponds to the Log-Euclidean mean
- Corresponds to the first definition of bi-invariant mean of [V. Arsigny, X. Pennec, and N. Ayache. Research Report RR-5885, INRIA, April 2006.]

Mean is stable by left / right composition and inversion

- If m is a mean of $\{g_i\}$ and h is any group element, then
 - $h \circ m$ is a mean of $\{h \circ g_i\}$,
 - $m \circ h$ is a mean of the points $\{g_i \circ h\}$
 - and $m^{(-1)}$ is a mean of $\{g_i^{(-1)}\}$

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

Bi-invariant Mean on Lie Groups

Fine existence

- If the data points belong to a sufficiently small normal convex neighborhood of some point, then there exists a unique solution in this NCN.
- Moreover, the iterated point strategy converges at least at a linear rate towards this unique solution, provided the initialization is close enough.
- Proof: using an auxiliary metric, the iteration is a contraction.

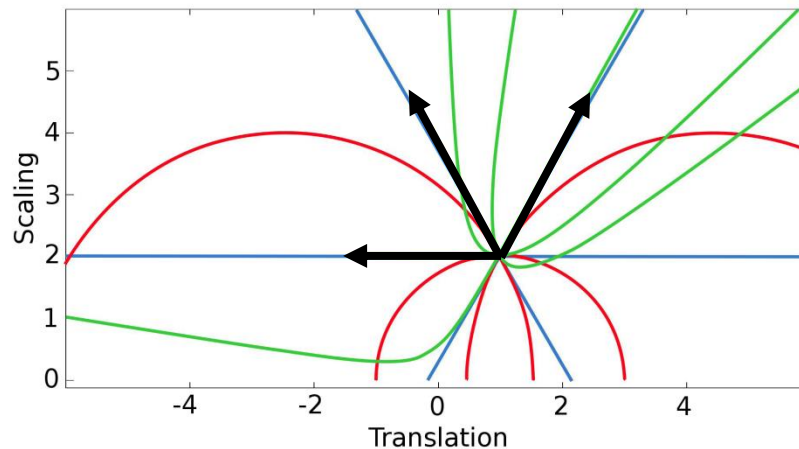
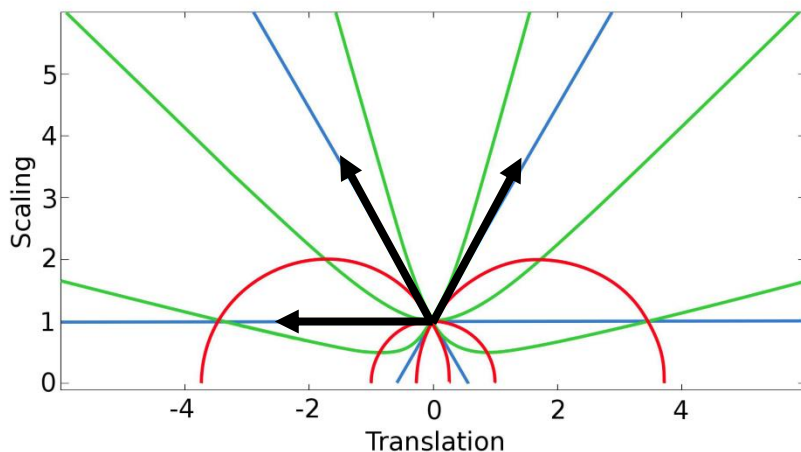
Closed-form for 2 points

- $m(t) = x \circ \text{Exp}(t \cdot \text{Log}(x^{(-1)} \circ y))$

Special Matrix Groups

Scaling and translations $ST(n)$

- No bi-invariant metric
- Group geodesics defined globally, all points are reachable
- Existence and uniqueness of bi-invariant mean (closed form)



Group / left-invariant / right-invariant geodesics

Special matrix groups

Heisenberg Group (resp. Scaled Upper Unitriangular Matrix Group)

- No bi-invariant metric
- Group geodesics defined globally, all points are reachable
- Existence and uniqueness of bi-invariant mean (closed form resp. solvable)

Rigid-body transformations

- Logarithm well defined iff log of rotation part is well defined, i.e. if the 2D rotation have angles $|\theta_i| < \pi$
- Existence and uniqueness with same criterion as for rotation parts (same as Riemannian)

SU(n) and GL(n):

- log does not always exist (need 2 exp to cover)

Example mean of 2D rigid-body transformation

$$T_1 = \left(\frac{\pi}{4}; -\frac{\sqrt{2}}{2}; \frac{\sqrt{2}}{2} \right) \quad T_2 = (0; \sqrt{2}; 0) \quad T_3 = \left(-\frac{\pi}{4}; -\frac{\sqrt{2}}{2}; -\frac{\sqrt{2}}{2} \right)$$

- Metric at Identity: $\text{dist}(Id, (\theta; t_1; t_2))^2 = \theta^2 + t_1^2 + t_2^2$
- Left-invariant Fréchet mean: $(0; 0; 0)$
- Log-Euclidean mean: $\left(0; \frac{\sqrt{2}-\pi/4}{3}; 0 \right) \simeq (0; 0.2096; 0)$
- Bi-invariant mean: $\left(0; \frac{\sqrt{2}-\pi/4}{1+\pi/4(\sqrt{2}+1)}; 0 \right) \simeq (0; 0.2171; 0)$
- Right-invariant Fréchet mean: $\left(0; \frac{\sqrt{2}}{3}; 0 \right) \simeq (0; 0.4714; 0)$

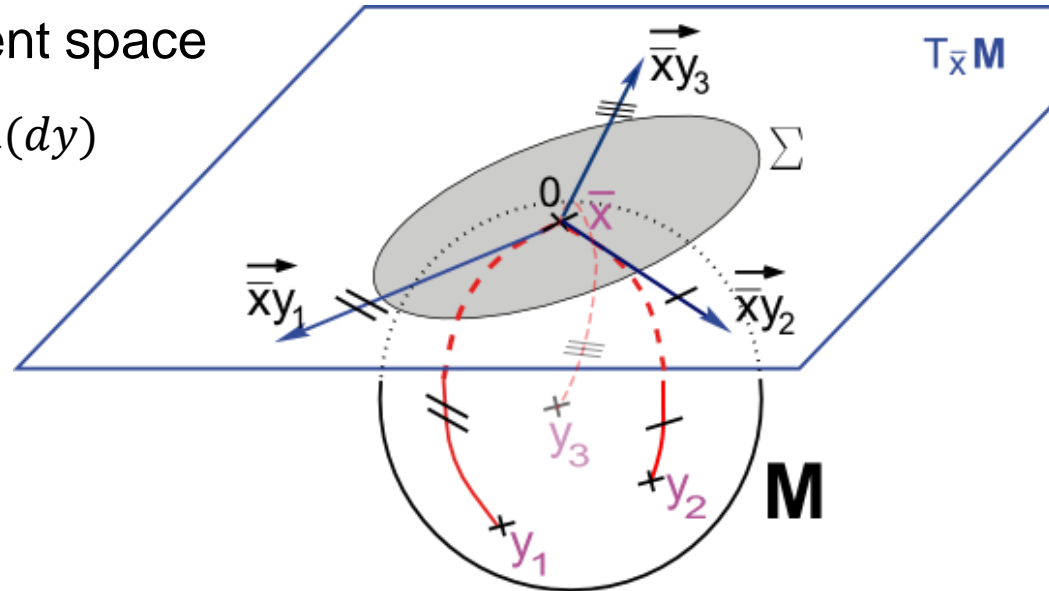
Generalization of the Statistical Framework

Covariance matrix & higher order moments

- Defined as tensors in tangent space

$$\Sigma = \int \text{Log}_x(y) \otimes \text{Log}_x(y) \mu(dy)$$

- Matrix expression changes according to the basis



Other statistical tools

- Mahalanobis distance well defined and bi-invariant

$$\mu_{(m,\Sigma)}(g) = \int [\text{Log}_m(g)]^i \Sigma_{ij}^{(-1)} [\text{Log}_m(g)]^j \mu(dy)$$

- ~~□ Tangent Principal Component Analysis (t-PCA)~~
- Principal Geodesic Analysis (PGA), provided a data likelihood
- Independent Component Analysis (ICA)

Cartan Connections vs Riemannian

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 (but no choice of metric to justify)
- The exponential does always not cover the full group
 - Pathological examples close to identity in finite dimension
 - In practice, similar limitations for the discrete Riemannian framework
- Global existence and uniqueness of bi-invariant mean?

Use a bi-invariant pseudo-Riemannian metric? [Miolane MaxEnt 2014]

What we gain

- A globally invariant structure invariant by composition & inversion
- Simple geodesics, efficient computations (stationarity, group exponential)
- The simplest linearization of transformations for statistics?

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

- Riemannian frameworks on Lie groups
- Lie groups as affine connection spaces
- Bi-invariant statistics with Canonical Cartan connection
- **The SVF framework for diffeomorphisms**

**Parallel transport to analyze Longitudinal deformations
Advances Statistics: CLT & PCA**

Riemannian Metrics on diffeomorphisms

Space of deformations

- Transformation $y = \phi(x)$
- Curves in transformation spaces: $\phi(x, t)$
- Tangent vector = speed vector field

$$v_t(x) = \frac{d\phi(x, t)}{dt}$$

Right invariant metric

- Eulerian scheme
- Sobolev Norm H_k or H_∞ (RKHS) in LDDMM \rightarrow diffeomorphisms [Miller, Trounev, Younes, Holm, Dupuis, Beg... 1998 – 2009]

$$\|v_t\|_{\phi_t} = \|v_t \circ \phi_t^{-1}\|_{Id}$$

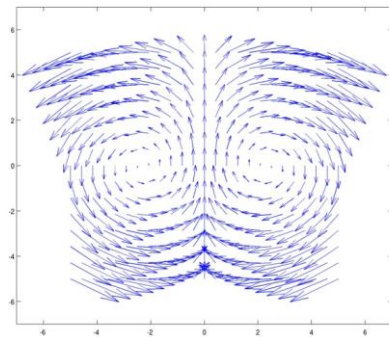
Geodesics determined by optimization of a time-varying vector field

- Distance
$$d^2(\phi_0, \phi_1) = \arg \min_{v_t} \left(\int_0^1 \|v_t\|_{\phi_t}^2 dt \right)$$
- Geodesics characterized by initial velocity / momentum
- Optimization for images is quite tricky (and lengthy)

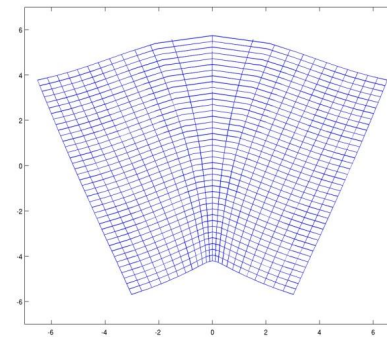
The SVF framework for Diffeomorphisms

Idea: [Arsigny MICCAI 2006, Bossa MICCAI 2007, Ashburner Neuroimage 2007]

- Exponential of a smooth vector field is a diffeomorphism
- Parameterize deformation by ~~time-varying~~ Stationary Velocity Fields



Stationary velocity field



Diffeomorphism

Direct generalization of numerical matrix algorithms

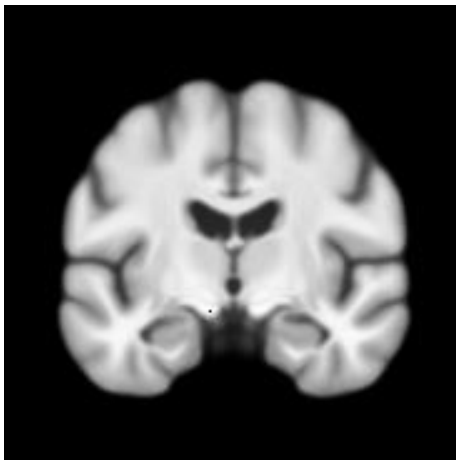
- Computing the deformation: **Scaling and squaring** [Arsigny MICCAI 2006]
recursive use of $\exp(\mathbf{v}) = \exp(\mathbf{v}/2) \circ \exp(\mathbf{v}/2)$
- Computing the Jacobian : $D\exp(\mathbf{v}) = D\exp(\mathbf{v}/2) \circ \exp(\mathbf{v}/2) \cdot D\exp(\mathbf{v}/2)$
- Updating the deformation parameters: **BCH formula** [Bossa MICCAI 2007]

$$\exp(\mathbf{v}) \circ \exp(\varepsilon \mathbf{u}) = \exp(\mathbf{v} + \varepsilon \mathbf{u} + [\mathbf{v}, \varepsilon \mathbf{u}]/2 + [\mathbf{v}, [\mathbf{v}, \varepsilon \mathbf{u}]]/12 + \dots)$$

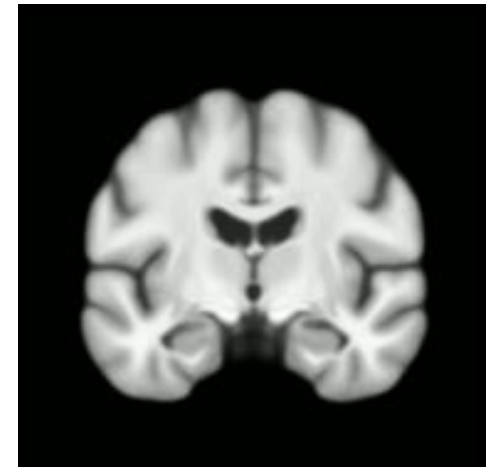
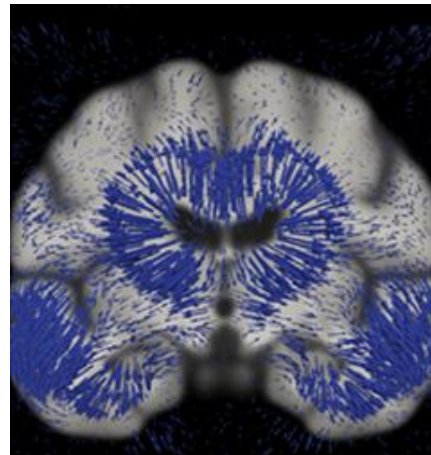
- Lie bracket $[\mathbf{v}, \mathbf{u}](p) = \text{Jac}(\mathbf{v})(p) \cdot \mathbf{u}(p) - \text{Jac}(\mathbf{u})(p) \cdot \mathbf{v}(p)$

Measuring Temporal Evolution with deformations

Optimize LCC with deformation parameterized by SVF



$$\varphi_t(x) = \exp(t \cdot v(x))$$



<https://team.inria.fr/asclepios/software/lcclogdemons/>

[Lorenzi, Ayache, Frisoni, Pennec, Neuroimage 81, 1 (2013) 470-483]

The Stationnary Velocity Fields (SVF) framework for diffeomorphisms

- SVF framework for diffeomorphisms is algorithmically simple
- Compatible with “inverse-consistency”
- Vector statistics directly generalized to diffeomorphisms.

Registration algorithms using log-demons:

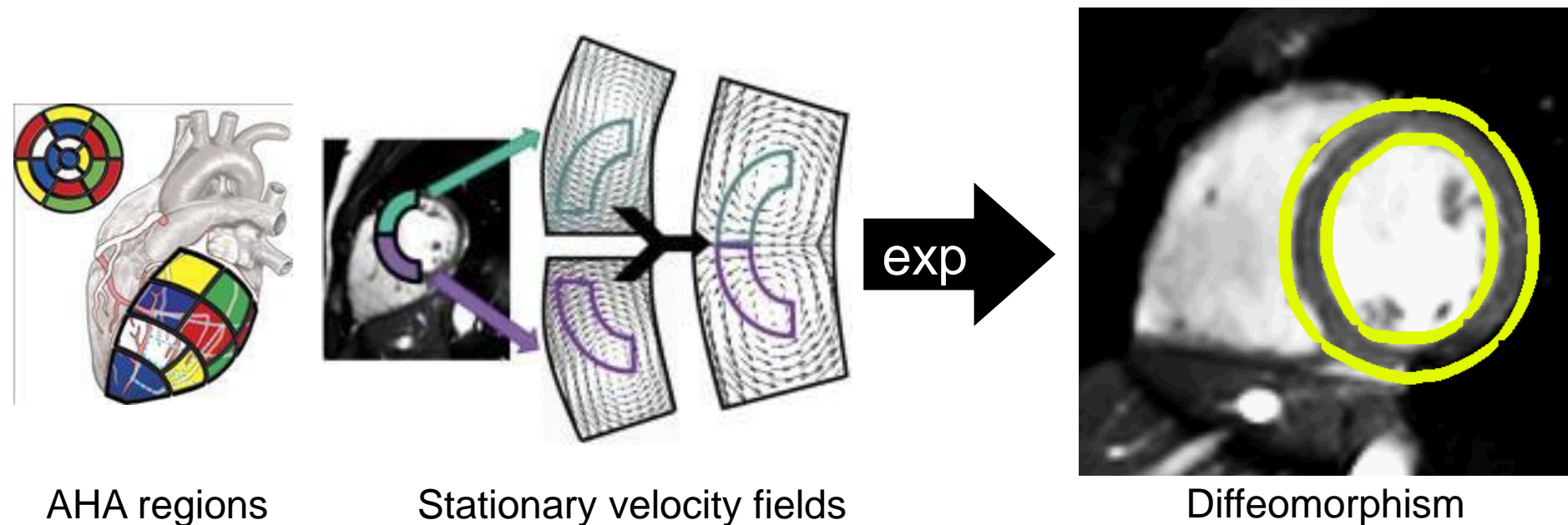
- Log-demons: Open-source ITK implementation (Vercauteren MICCAI 2008)
<http://hdl.handle.net/10380/3060>
[MICCAI Young Scientist Impact award 2013]
- Tensor (DTI) Log-demons (Sweet WBIR 2010):
<https://gforge.inria.fr/projects/ttk>
- LCC log-demons for AD (Lorenzi, Neuroimage. 2013)
<https://team.inria.fr/asclepios/software/lcclogdemons/>
- 3D myocardium strain / incompressible deformations (Mansi MICCAI'10)
- Hierarchical multiscale polyaffine log-demons (Seiler, Media 2012)
<http://www.stanford.edu/~cseiler/software.html>
[MICCAI 2011 Young Scientist award]

A powerful framework for statistics

Parametric diffeomorphisms [Arsigny et al., MICCAI 06, JMIV 09]

- One affine transformation per region (polyaffines transformations)
- Cardiac motion tracking for **each subject** [McLeod, Miccai 2013]

Log demons projected but with 204 parameters instead of a few millions



AHA regions

Stationary velocity fields

Diffeomorphism

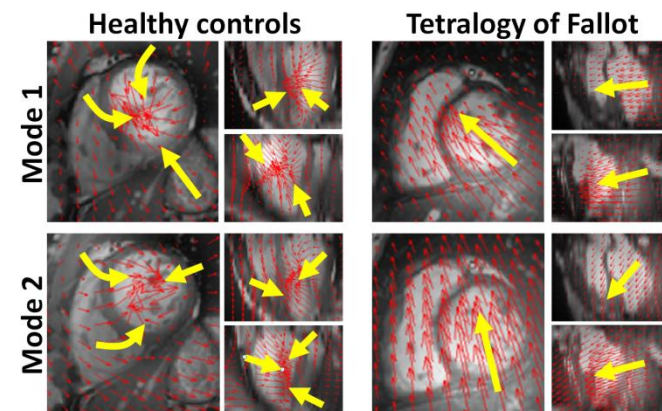
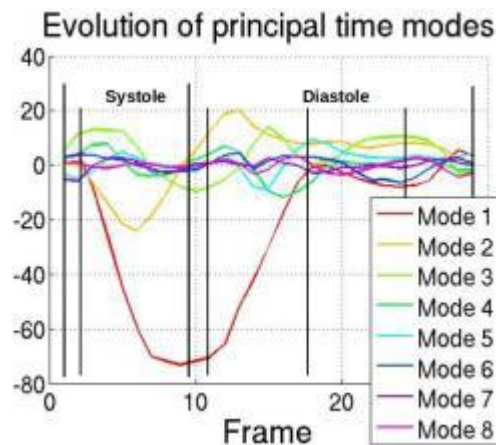
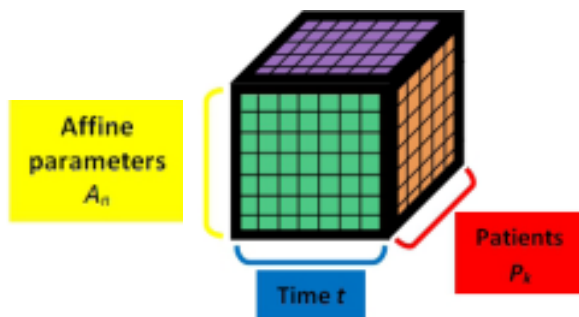
A powerful framework for statistics

Parametric diffeomorphisms [Arsigny et al., MICCAI 06, JMIV 09]

- One affine transformation per region (polyaffines transformations)
- Cardiac motion tracking for **each subject** [McLeod, Miccai 2013]

Log demons projected but with 204 parameters instead of a few millions

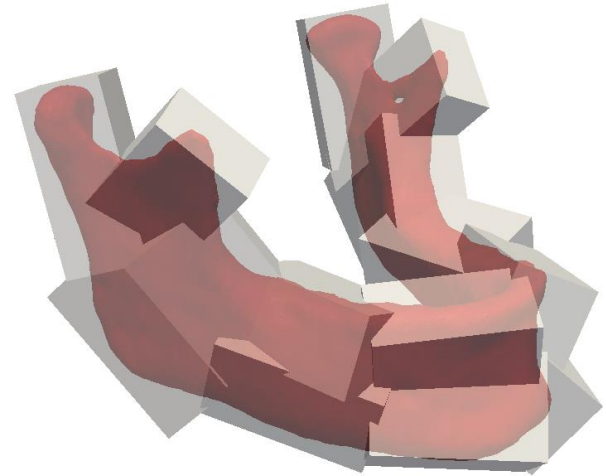
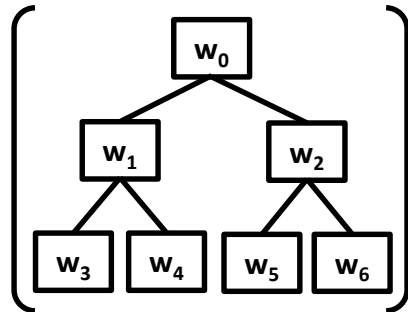
- **Group analysis** using tensor reduction : reduced model
8 temporal modes x 3 spatial modes = 24 parameters (instead of 204)



Hierarchical Deformation model

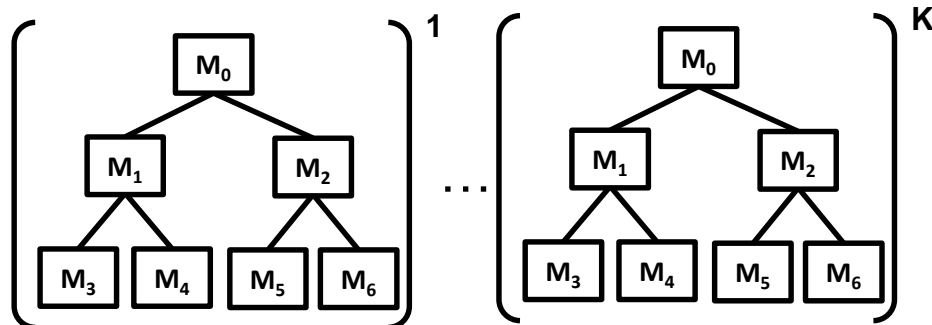
Population level:

Spatial structure of the anatomy common to all subjects

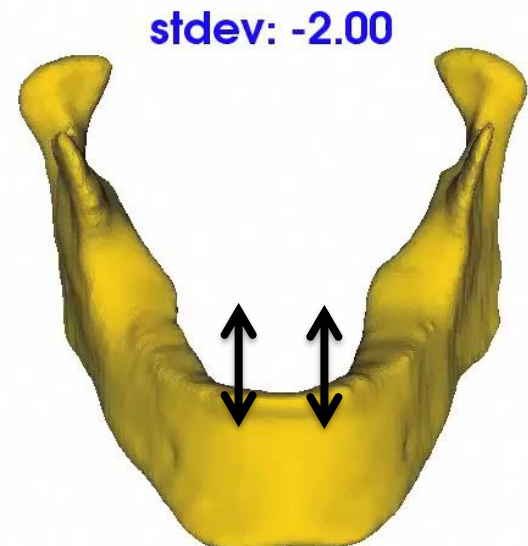


Subject level:

Varying deformation atoms for each subject



Aff(3) valued trees



Hierarchical Estimation of the Variability

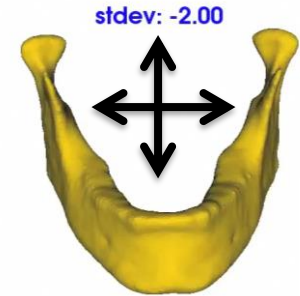
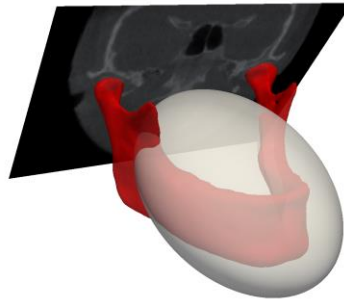
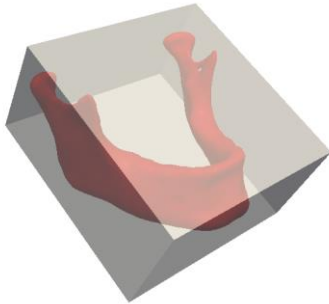
Oriented bounding boxes

Weights

Structure

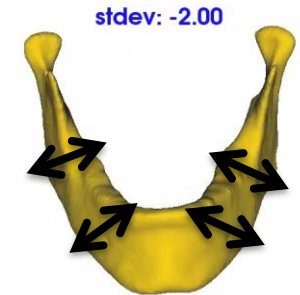
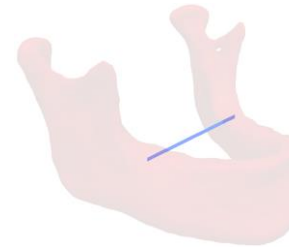
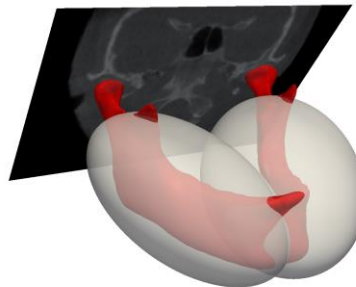
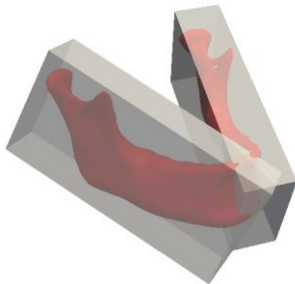
First mode of variation

Level 0



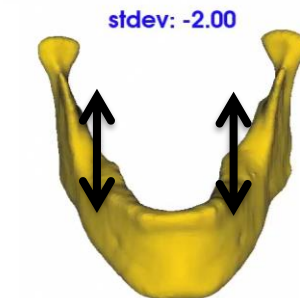
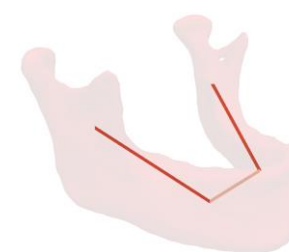
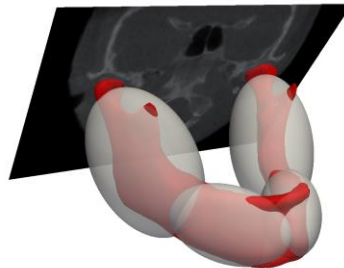
Global scaling

Level 1



Thickness

Level 2

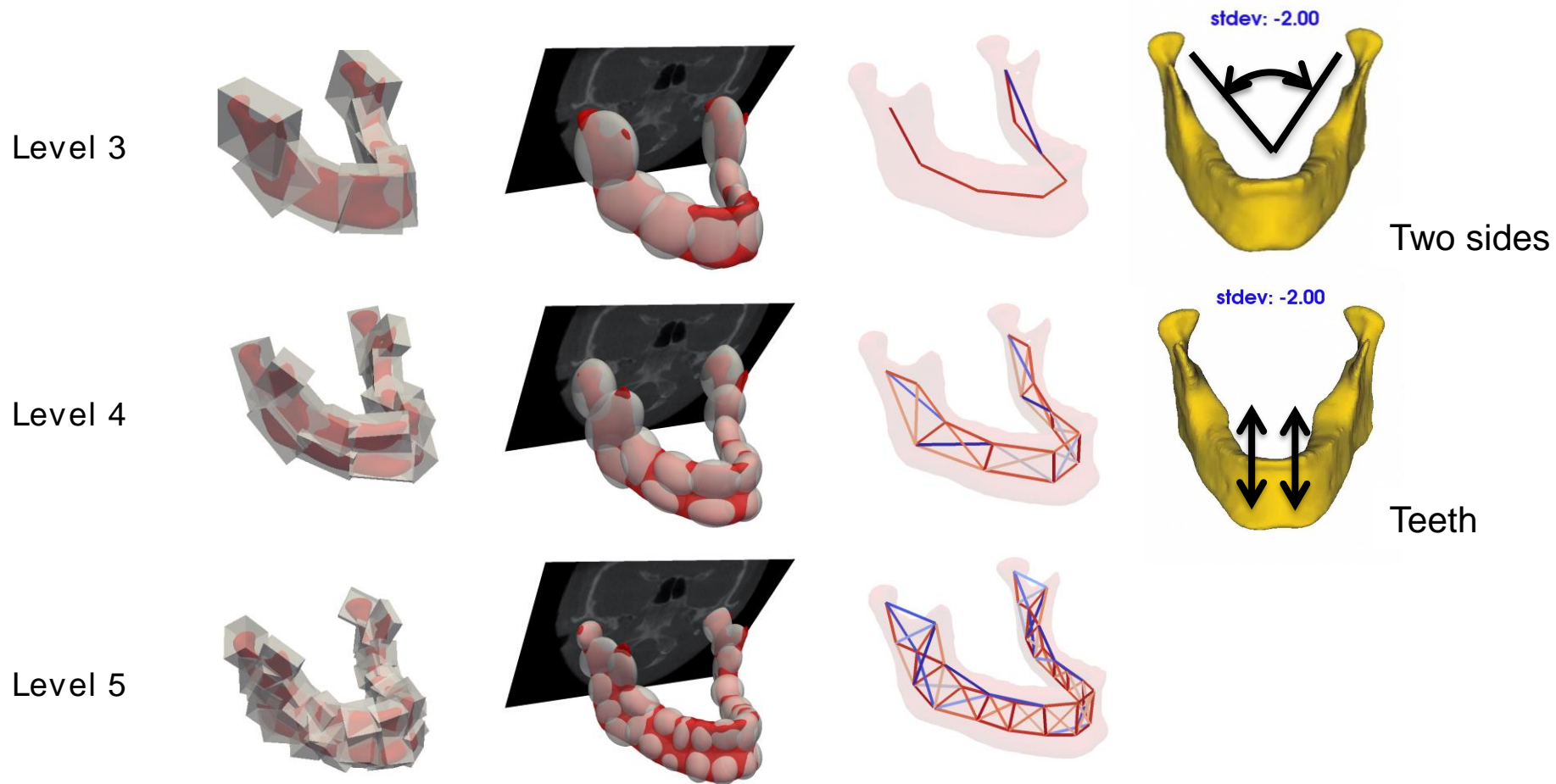


Angle and ramus

47 subjects

[Seiler, Pennec, Reyes, Medical Image Analysis 16(7):1371-1384, 2012]

Hierarchical Estimation of the Variability



47 subjects

[Seiler, Pennec, Reyes, *Medical Image Analysis* 16(7):1371-1384, 2012]

References for Statistics on Manifolds and Lie Groups

Statistics on Riemannian manifolds

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

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

- 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>

Bi-invariant means with Cartan connections on Lie groups

- Xavier Pennec and Vincent Arsigny. Exponential Barycenters of the Canonical Cartan Connection and Invariant Means on Lie Groups. In Frederic Barbaresco, Amit Mishra, and Frank Nielsen, editors, *Matrix Information Geometry*, pages 123-166. Springer, May 2012. <http://hal.inria.fr/hal-00699361/PDF/Bi-Invar-Means.pdf>

Cartan connexion for diffeomorphisms:

- Marco Lorenzi and Xavier Pennec. Geodesics, Parallel Transport & One-parameter Subgroups for Diffeomorphic Image Registration. *International Journal of Computer Vision*, 105(2), November 2013 <https://hal.inria.fr/hal-00813835/document>