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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.

2/ Metric and Affine Geometric Settings for Lie Groups

ESI semester Infinite-dimensional Geometry: Theory and Applications Week 5, 02/2025

Geometric Statistics: Mathematical foundations and applications in computational anatomy

Intrinsic Statistics on Riemannian Manifolds

Metric and Affine Geometric Settings for Lie Groups

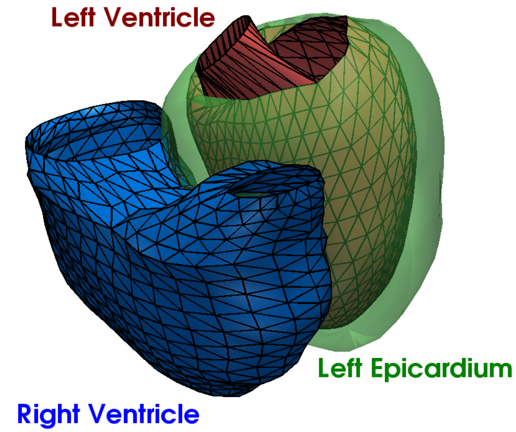
- Riemannian frameworks on Lie groups
- Lie groups as affine connection spaces
- The SVF framework for diffeomorphisms
- Longitudinal modeling with parallel transport

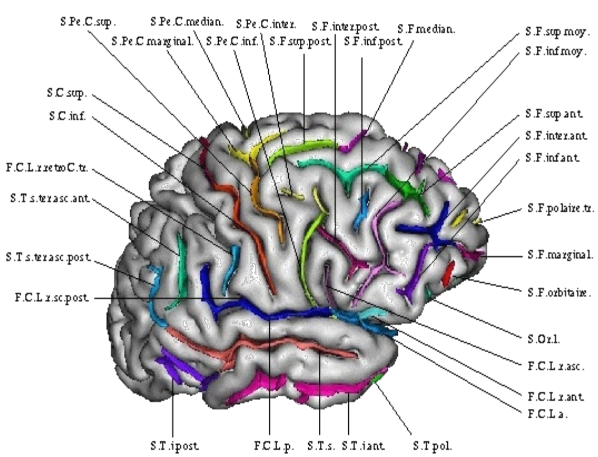
Advances Statistics: CLT & PCA

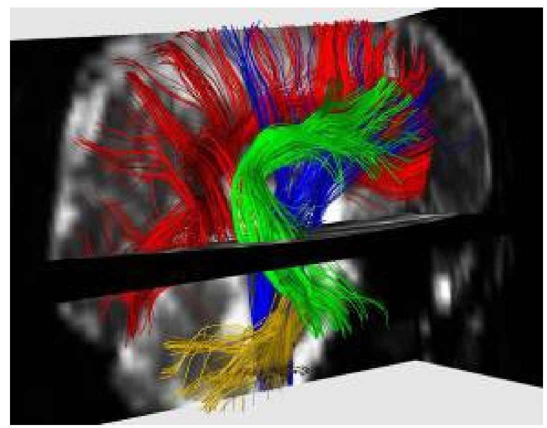
Geometric features in Computational Anatomy

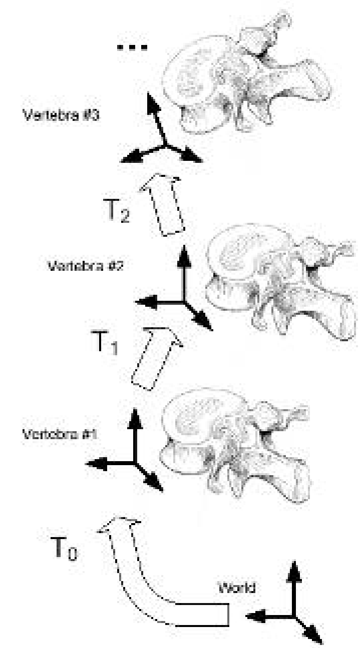
Noisy geometric features

- Curves, sets of curves (fiber tracts)
- Surfaces, SPD matrices
- Transformations









Statistical modeling at the population level

- Simple Statistics on non-linear manifolds?
  - Mean, covariance of its estimation, PCA, PLS, ICA

Exp_x / Log_x and Fréchet mean are the basis of algorithms to compute on Riemannian/affine manifolds

~~Minimal # of non-linear charts~~ → one chart per point!

- Normal coordinate system = most linear chart at each point

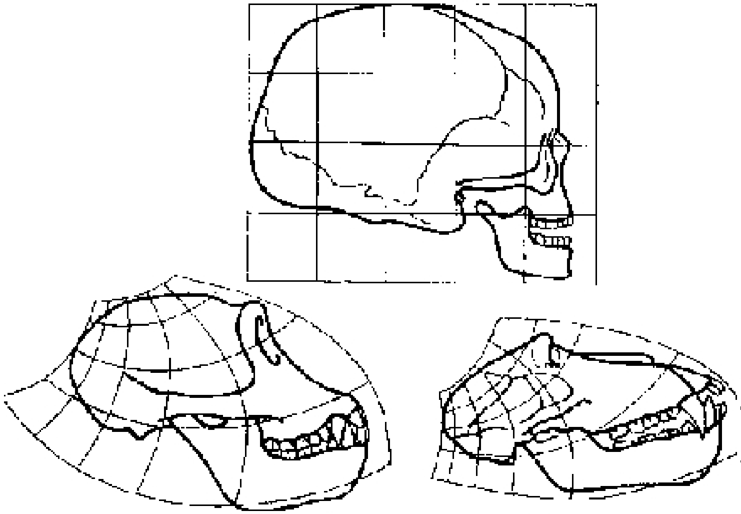
Simple statistics

- Mean through an exponential barycenter iteration
- Covariance matrices and higher order moments
- Tangent PCA or more complex PGA / BSA

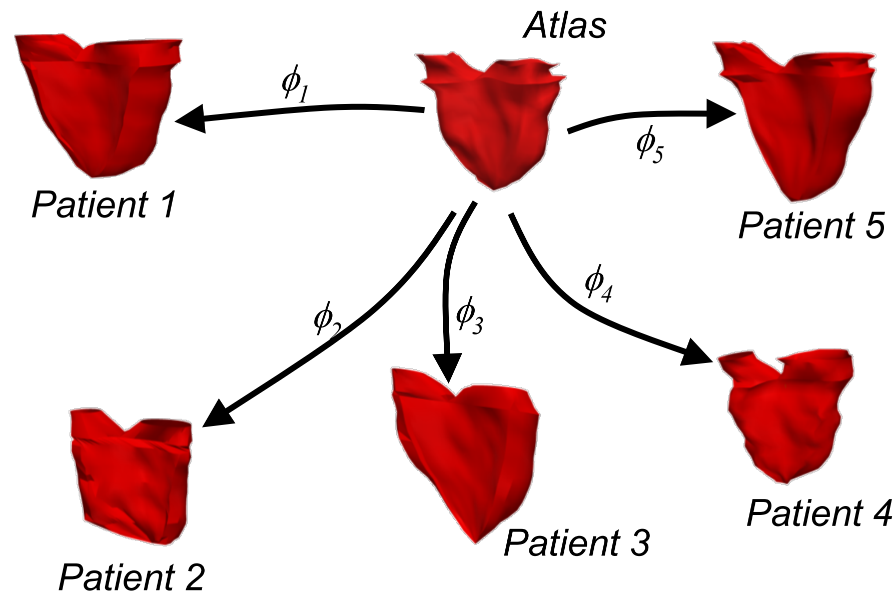
Manifold-valued image processing [XP, IJCV 2006]

- Interpolation / filtering / convolution: weighted means
- Diffusion, extrapolation:
  Discrete Laplacian in tangent space = Laplace-Beltrami

Morphometry through Deformations



Skulls of a human, a chimpanzee and a baboon
and transformations between them



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

- Template / atlas shape plays the role of the mean
- Observation = "random" deformation of a reference template
- Lift differences to transformation group for statistical analyses
  - **Statistical framework compatible with group operations?**

Natural Riemannian Metrics on Transformations

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

- Composition g o h and inversion g^{-1} are smooth
- Left and Right translation $L_g(f) = g \circ f \quad R_g(f) = f \circ g$
- Conjugation $\mathrm{Conj}_g(f) = g \circ f \circ g^{-1}$
- Symmetry: $S_g(f) = g \circ f^{-1} \circ g$

Natural Riemannian metric choices

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

Implementation

- Practical computations using left (or right) translations

$$\mathrm{Exp}_f(x) = f \circ \mathrm{Exp}_{Id}(DL_{f^{(-1)}} .x) \qquad \overrightarrow{fg} = \mathrm{Log}_f(g) = DL_f .\mathrm{Log}_{Id}(f^{(-1)} \circ g)$$

General Non-Compact and Non-Commutative case

No Bi-invariant Mean for 2D Rigid Body Transformations

- Metric at Identity: $dist(Id,(\theta;t_1;t_2))^2 = \theta^2 + t_1^2 + t_2^2$
- $T_1 = \left(\frac{\pi}{4};\ -\frac{\sqrt{2}}{2};\frac{\sqrt{2}}{2}\right) \quad T_2 = \left(0;\ \sqrt{2};0\ \right) \quad T_3 = \left(-\frac{\pi}{4};\ -\frac{\sqrt{2}}{2};-\frac{\sqrt{2}}{2}\right)$
- Left-invariant Fréchet mean: $(0;0;0\ )$
- Right-invariant Fréchet mean: $\left(0;\frac{\sqrt{2}}{3};0\right) \simeq (0;0.4714;0)$
- **Incompatibility of the Fréchet mean with the group structure**

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?**

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Special curves on 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: $\gamma_x(s+t) = \gamma_x(s).\,\gamma_x(t)$

Lie group exponential

- Definition: $x \in \mathfrak{g} \rightarrow Exp(x) = \gamma_x(1) \in G$
- 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

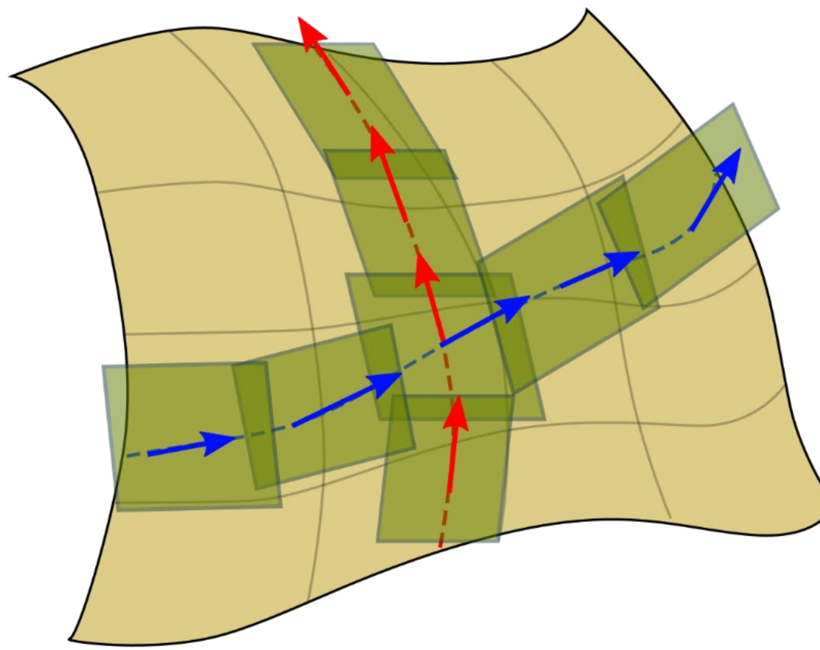
- Left / Right-invariant geodesics, one-parameter subgroups

Question: Can one-parameter subgroups be geodesics?

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



Adapted from Lê Nguyên Hoang, science4all.org

Geodesics = straight lines

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

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

Left invariant connections $\nabla_{DL.X} DL.Y = DL.\nabla_X Y$

- Characterized by bilinear form on the Lie algebra $a(x,y) = \nabla_{\tilde{X}} \tilde{Y}|_e \in \mathfrak{g}$ for left-invariant vector fields, use linearity + Leibnitz rule for other vf
- Symmetric part $\frac{1}{2}(a(x,y) + a(y,x))$ specifies geodesics
- Skew symmetric part $\frac{1}{2}(a(x,y) - a(y,x))$ specifies torsion along them

Bi-invariant connections

- $a(Ad(g).x, Ad(g).y) = Ad(g).a(x,y)$
- $a([z,x],y) + a(x,[z,y]) = [z, a(x,y)], \;\; \mathrm{x, y, z \; in} \;\; \mathfrak{g}$

Cartan Schouten connections (def. of Postnikov)

- Left-Inv connections for which one-parameter subgroups are geodesics
- Uniquely determined by $a(x,x) = 0$ (skew symmetry)

Canonical Cartan connections on Lie groups

Bi-invariant Cartan Schouten connections

- Family $a(x,y) = \lambda[x,y]$ (-,0, + connections for λ=0,1/2,1)
  - Turner Laquer 1992: all of them for compact simple Lie groups except SU(n) (2-d family)
- Same group geodesics ($a(x,y) + a(y,x) = 0$):
  one-parameter subgroups and their left and right translations
- Curvature: $\mathrm{R}(x,y) = \lambda(\lambda-1)[[x,y],z]$
- Torsion: $T(x,y) = 2a(x,y) - [x,y]$

Left/Right Cartan-Schouten Connection (λ=0/λ=1)

- Flat space with torsion (absolute parallelism)
- Left (resp. Right)-invariant vector fields are covariantly constant
- Parallel transport is left (resp. right) translation

Unique symmetric bi-invariant Cartan connection (λ=1/2)

- $a(x,y) = \frac{1}{2}[x,y]$
- Curvature $R(x,y)z = -\frac{1}{4}[[x,y],z]$
- Parallel transport along geodesics: $\Pi_{\exp(y)}x = DL_{\exp(\frac{y}{2})}.\ DL_{\exp(\frac{y}{2})}$.x

Cartan Connections are generally not metric

Levi-Civita Connection of a left-invariant (pseudo) metric is left-invariant

- Metric dual of the bracket $< ad^* (x, y), z > = < [x, z], y >$
- $a(x, y) = \frac{1}{2}[x, y] - \frac{1}{2}\left(ad^*(x, y) + ad^*(y, x)\right)$

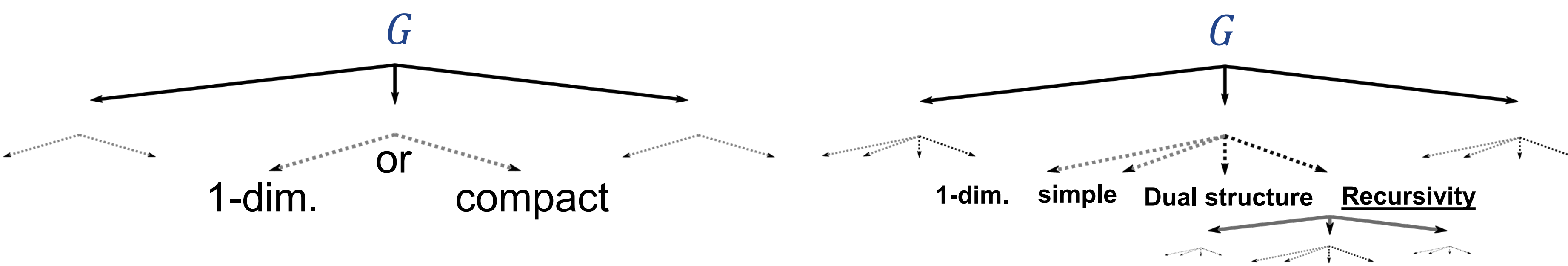
Bi-invariant (pseudo) metric => Symmetric Cartan connection

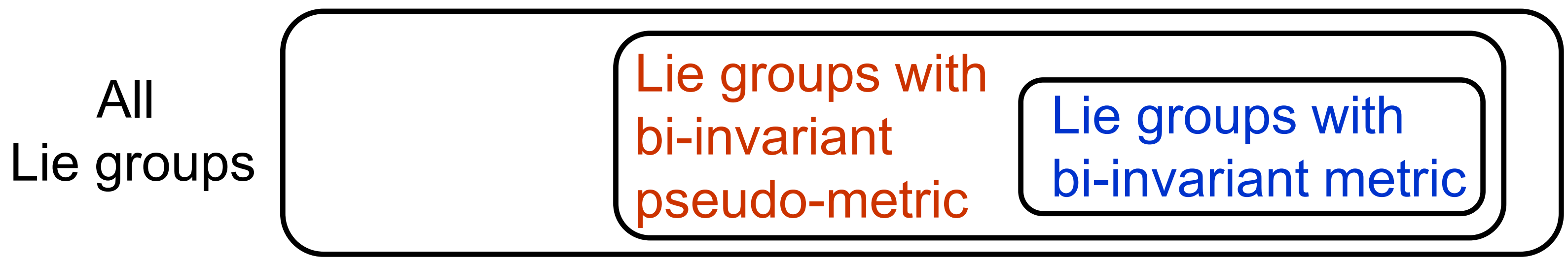
- A left-invariant (pseudo) metric is right-invariant if it is Ad-invariant
$$< x, y > = < Ad_g(x), Ad_g(y) >$$
- Infinitesimally: $< [x, z], y > + < x, [y, z] > = 0$ or $ad^*(x, y) + ad^*(y, x) = 0$

Existence of bi-invariant (pseudo) metrics

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

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





[Miolane, XP, 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**

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 exp)
- Other geodesics by left or right translation
  - 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

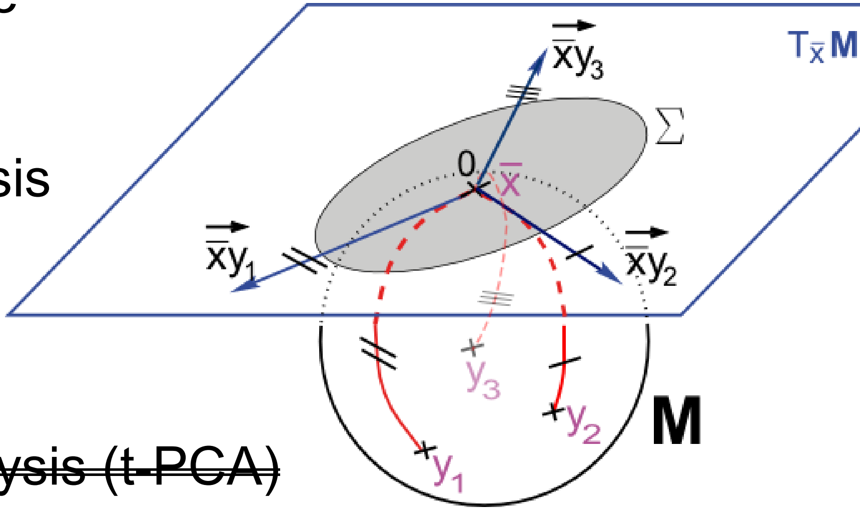
- $\sum_i Log_x(y_i) = 0$ [Emery, Mokobodzki 91, Corcuera, Kendall 99]
- Existence **local uniqueness** if local convexity [Arnaudon & Li, 2005]

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, chi² 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 $\sum Log\left(x^{-1}.y_i\right) = 0$
- 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**

m = mean$\{g\}$ $\Longrightarrow$ $h \circ m$ = mean$\{h \circ g_i\}$, $m \circ h$ = mean$\{g_i \circ h\}$ and $m^{(-1)}$ = mean$\left\{g_i^{(-1)}\right\}$

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]

Example mean of 2D rigid-body transformation

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

- Metric at Identity: $dist(Id,(\theta;t_1;t_2))^2 = \theta^2 +\ t_1^2 + t_2^2$
- 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: $\left(0;\frac{\sqrt{2}}{3};0\right) \simeq (0;0.4714;0)$

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

What we gain with Cartan-Schouten connection

- A globally invariant structure invariant by composition & inversion
- Simple geodesics, efficient computations (stationarity, group exponential)
- Consistency with any bi-invariant (pseudo)-metric
- The simplest linearization of transformations for statistics on Lie groups?

Geometric Statistics: Mathematical foundations and applications in computational anatomy

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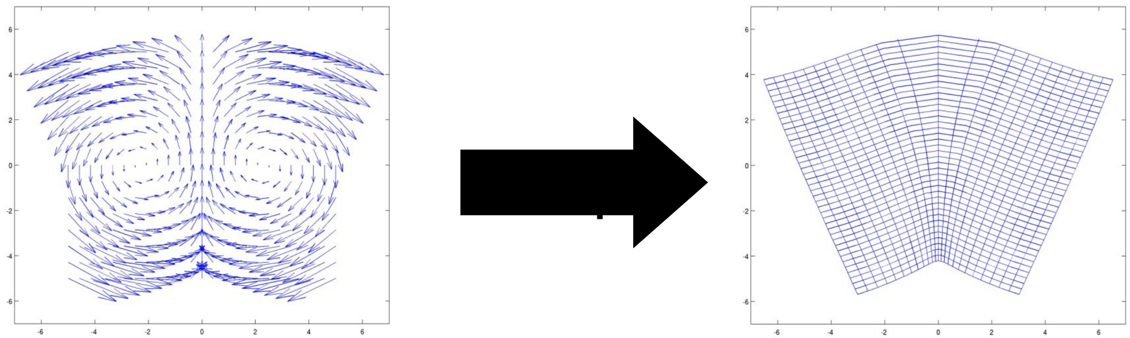
Advances Statistics: CLT & PCA

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



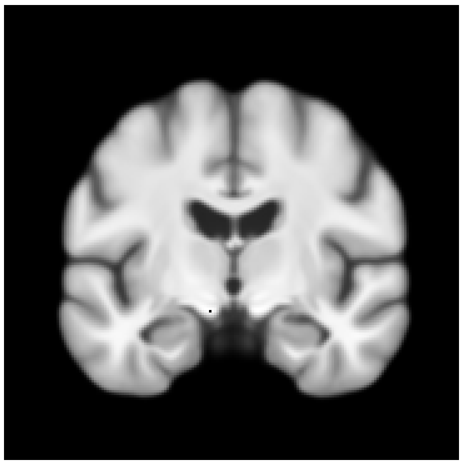
Stationary velocity field — Diffeomorphism

Efficient numerical algorithms

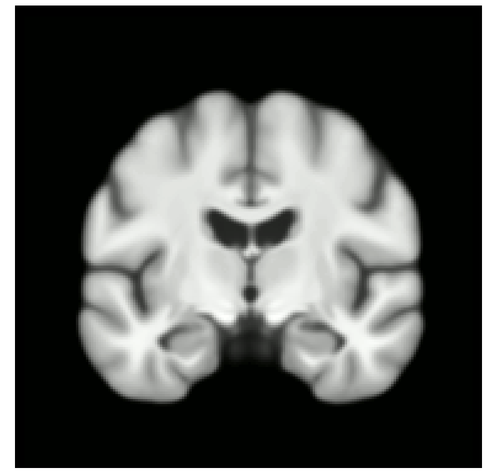
- Recursive **Scaling and squaring algorithm** **[Arsigny MICCAI 2006]**
  - Deformation: exp($\boldsymbol{v}$)=exp($\boldsymbol{v}$/2) o exp($\boldsymbol{v}$/2)
  - Jacobian: Dexp(v) = Dexp(v/2) o exp(v/2) . Dexp(v/2)
- Optimize deformation parameters: **BCH formula** **[Bossa MICCAI 2007]**
  - $\exp(\boldsymbol{v}) \circ \exp(\varepsilon \boldsymbol{u}) = \exp(\boldsymbol{v} + \varepsilon \boldsymbol{u} + [\boldsymbol{v}, \varepsilon \boldsymbol{u}]/2 + [\boldsymbol{v},[\boldsymbol{v}, \varepsilon \boldsymbol{u}]]/12 + \ldots)$ where $[\boldsymbol{v},\boldsymbol{u}](p) = \mathrm{Jac}(\boldsymbol{v})(p).\boldsymbol{u}(p) - \mathrm{Jac}(\boldsymbol{u})(p).\boldsymbol{v}(p)$

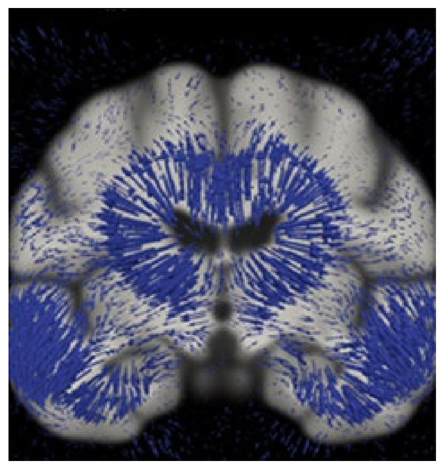
Measuring Temporal Evolution with deformations: Deformation-based morphometry

Fast registration with deformation parameterized by SVF



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





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

[LCC log-demons for longitudinal brain imaging.
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:

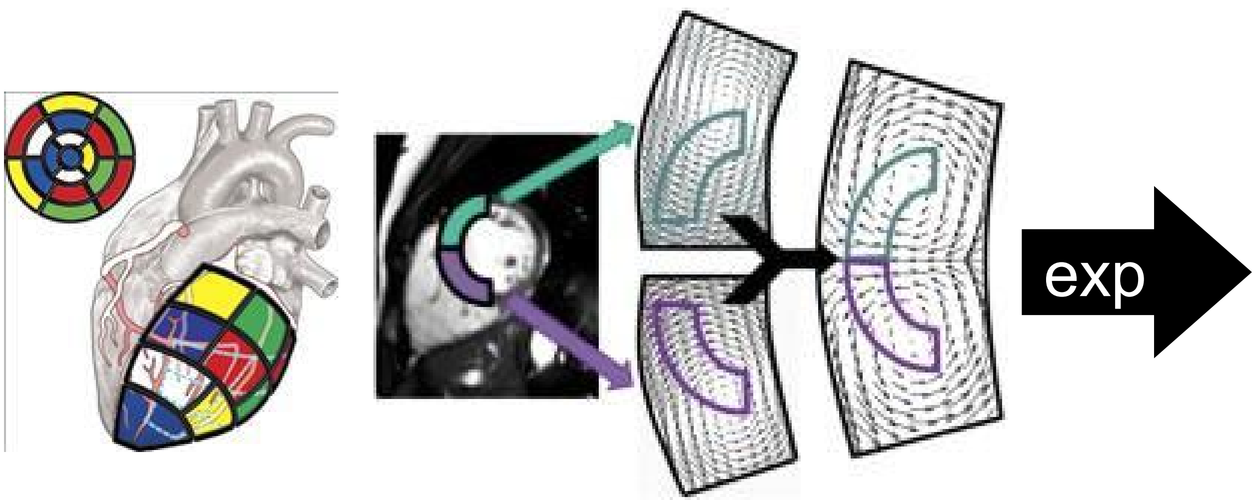
- Log-demons: Open-source ITK implementation (Vercauteren MICCAI 2008)
  http://hdl.handle.net/10380/3060 [MICCAI 2013 Young Scientist award]
- Tensor (DTI) Log-demons (Sweet WBIR 2010):
  https://gforge.inria.fr/projects/ttk
- LCC log-demons for AD (Lorenzi, Neuroimage. 2013)
  https://team.inria.fr/asclepios/software/lcclogdemons/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

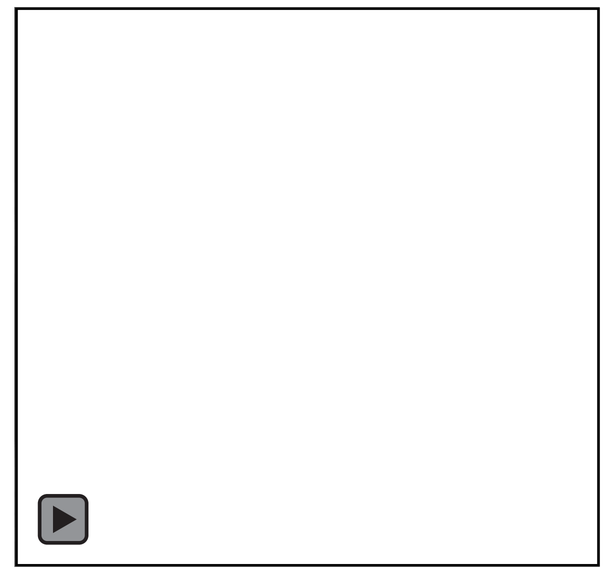
A powerful framework for statistics

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 with 204 parameters [McLeod, Miccai 2013]

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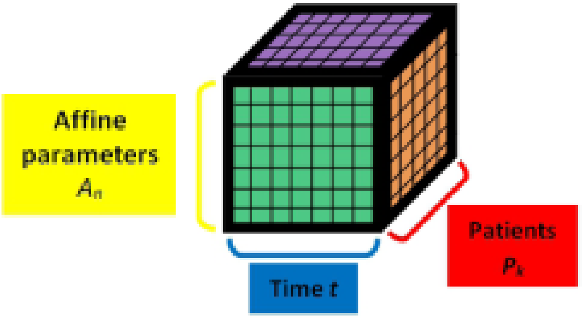
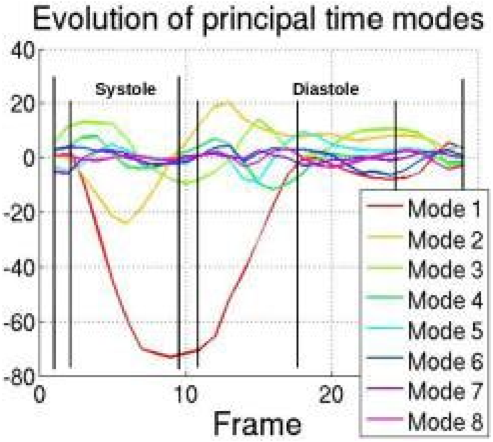
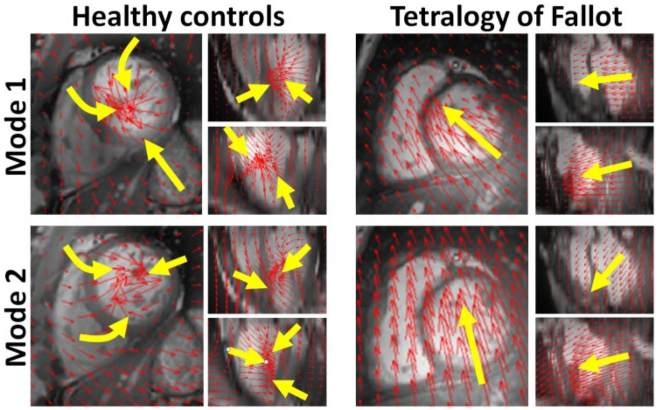
Log demons projected but with 204 parameters instead of a few millions

- **Group analysis** using tensor reduction : reduced model

8 temporal modes x 3 spatial modes = 24 parameters (instead of 204)







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- Perspectives

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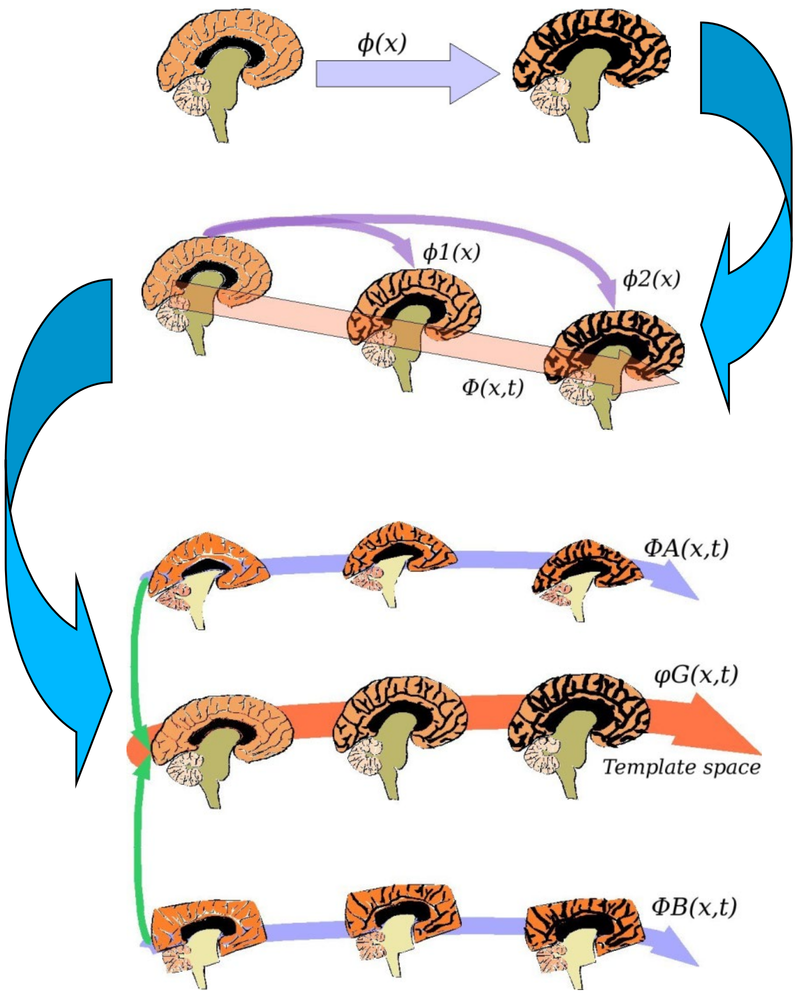
Analysis of longitudinal datasets



Single-subject, two time points

Log-Demons (LCC criteria)

Single-subject, multiple time points

4D registration of time series within the Log-Demons registration: geodesic regression

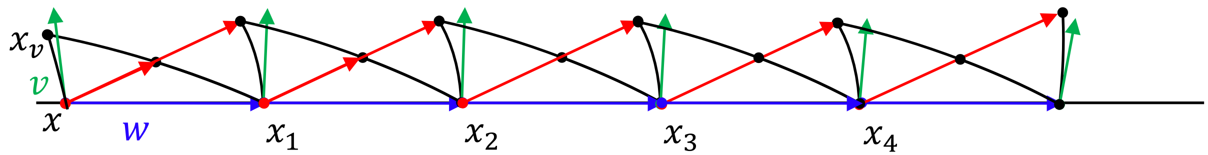
Multiple subjects, multiple time points

Population trend with parallel transport of SVF along inter-subject trajectories

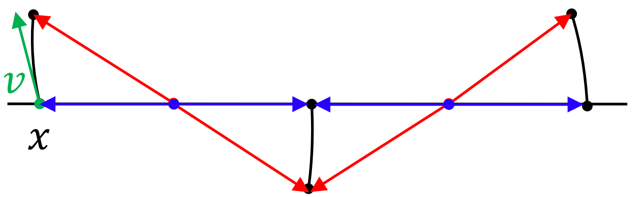
[Lorenzi et al, IPMI 2011, JMIV 2013]

Discrete approximations of Parallel transport

Schild's Ladder [Lecture at Princeton 60ies, Elhers et al 1972]



- Build geodesic parallelogram
- Iterate along the curve
- One step is a 1st order approximation **[Kheyfets et al 2000]**



Pole ladder: [Lorenzi, XP, JMIV 50 (1-2), 2013]

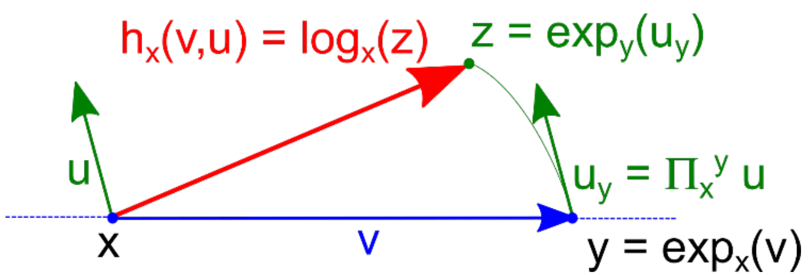
- Simpler method with piecewise geodesics
  - Closed form expression for Cartan connection on Lie groups

→ No approximation formula beyond 1st order for SL
→ No results for the iterated SL and PL schemes
→ No results for approximate geodesics

Taylor expansion of geodesic triangles

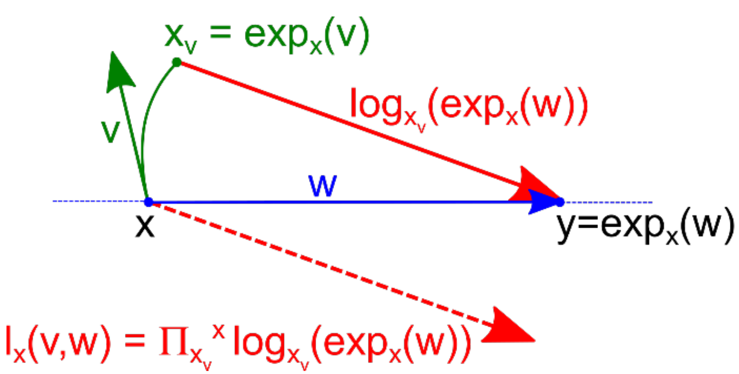
Key idea: use parallel transport rather that normal chart to relate $T_x M$ to $T_{x_v} M$

Gavrilov's double exponential is a tensorial series (2006):



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

Neighboring log expansion [XP arXiv:1906.07418, 2019]



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

Torsion free affine manifolds

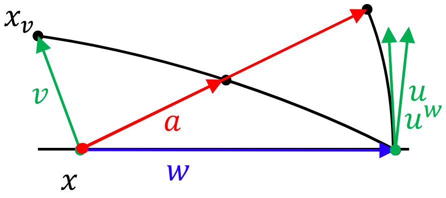
Convergence of Schild's Ladder

Gavrilov's Taylor expansion of one Schild's ladder step

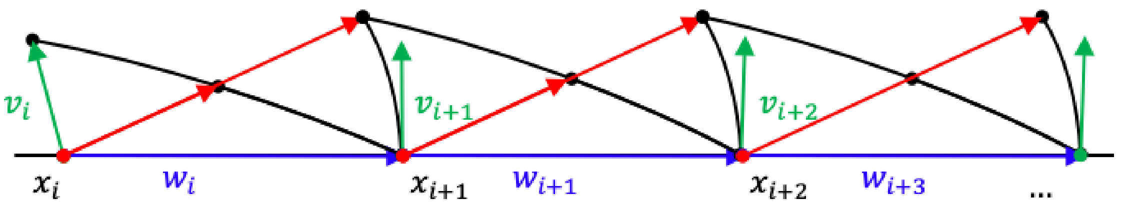
- A new Taylor series for mid-point rule

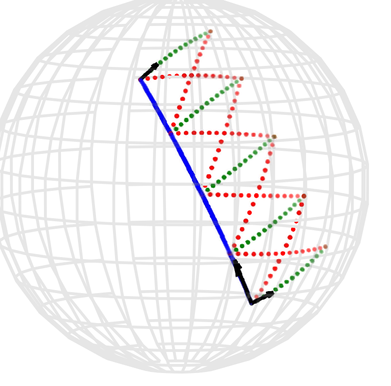
$$2a = w + v + \frac{1}{6}R(v,w)(w-v) + O(4)$$

$$u - u^w = \frac{1}{2}R(w,v)v + O(4)$$



Convergence of the iterated Schild's ladder





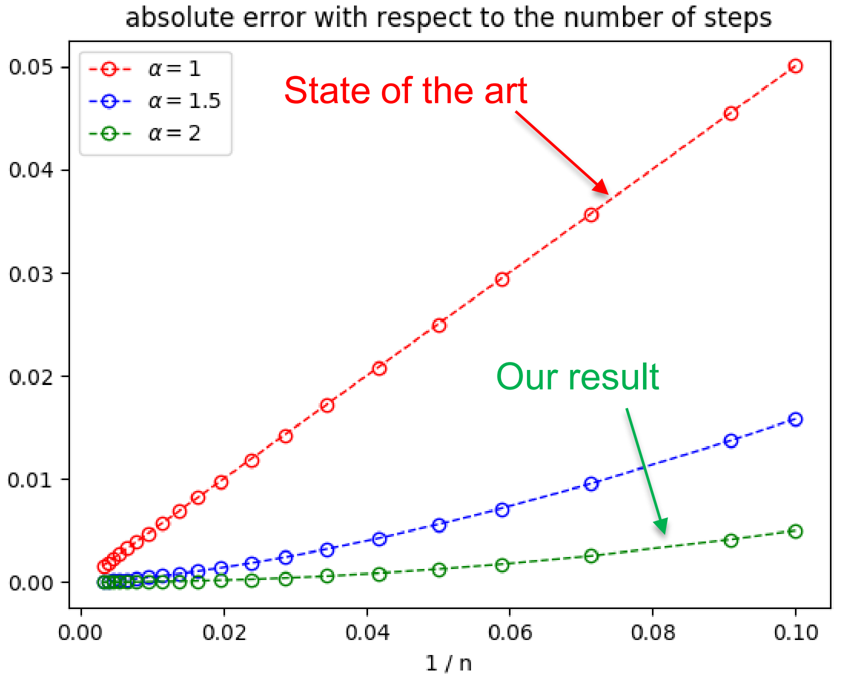
$$v_{i+1} = n^\alpha \cdot \mathrm{schild}(x_i, \frac{w_i}{n}, \frac{v_i}{n^\alpha}),$$

Theorem: the scheme converge at speed $\|v_n - \Pi_x^{x_n} v\| \leq \frac{\tau}{n^\alpha} + \frac{\beta}{n^2}.$

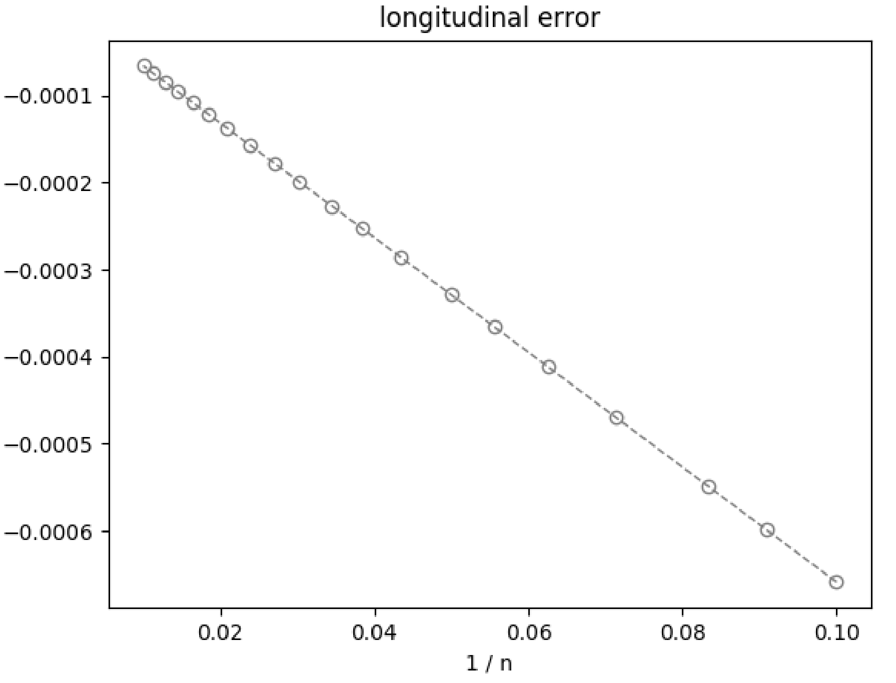
[N. Guigui, XP, Numerical Accuracy of Ladder Schemes for Parallel Transport on Manifolds. Foundations of Computational Mathematics, 22:757-790, 06-2022. Arxiv 2007.07585.]

Convergence of Schild's Ladder

Numerical experiments in controlled spaces



Simulations on the sphere:
constant curvature



Simulations on the space of SPD
matrices: negative curvature

[N. Guigui, XP, Numerical Accuracy of Ladder Schemes for Parallel Transport on Manifolds. Foundations of Computational Mathematics, 22:757-790, 06-2022. Arxiv 2007.07585.]

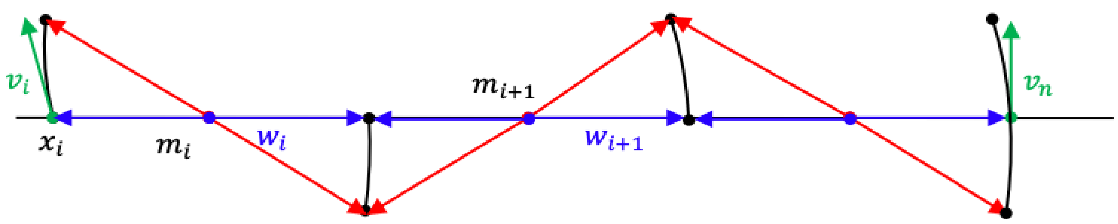
Convergence of pole Ladder

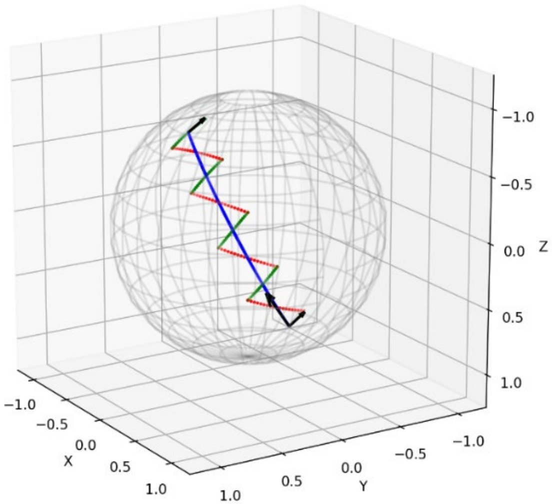
Taylor expansion of one pole ladder step

- One step is of order 4 in affine manifolds **[XP, Arxiv 1805.11436, 2018]**
- **Exact in symmetric spaces (transvection)!**

$$\text{pole(u)} = \Pi(u) + \frac{1}{12}\nabla_v R(u,v)(5u-2v) + \frac{1}{12}\nabla_u R(u,v)(v-2u) + O(5)$$

Convergence of the iterated pole ladder





Theorem: the scheme converge at speed $\left\|v_n - \Pi_m^{m_n} v\right\| \leq \frac{\gamma}{n^2}$

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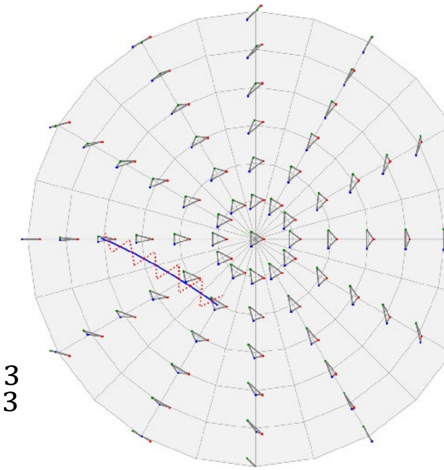
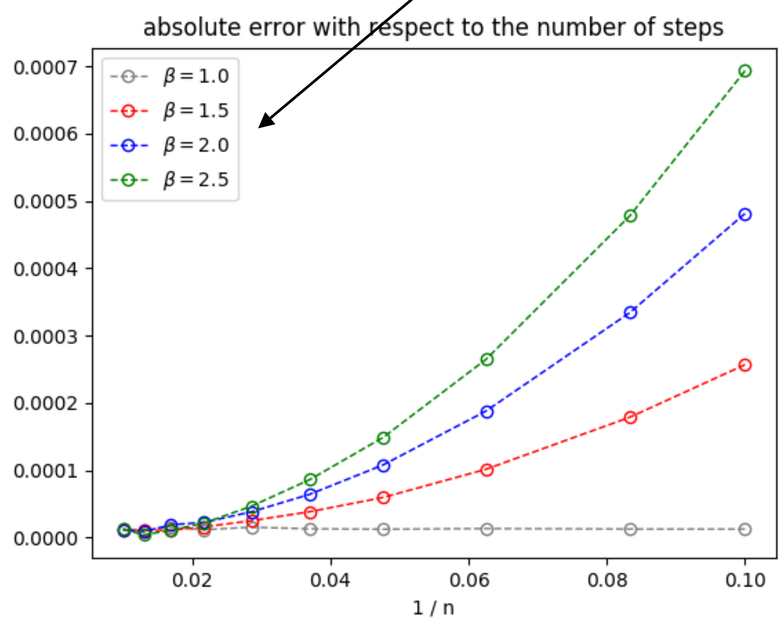
Convergence of pole Ladder

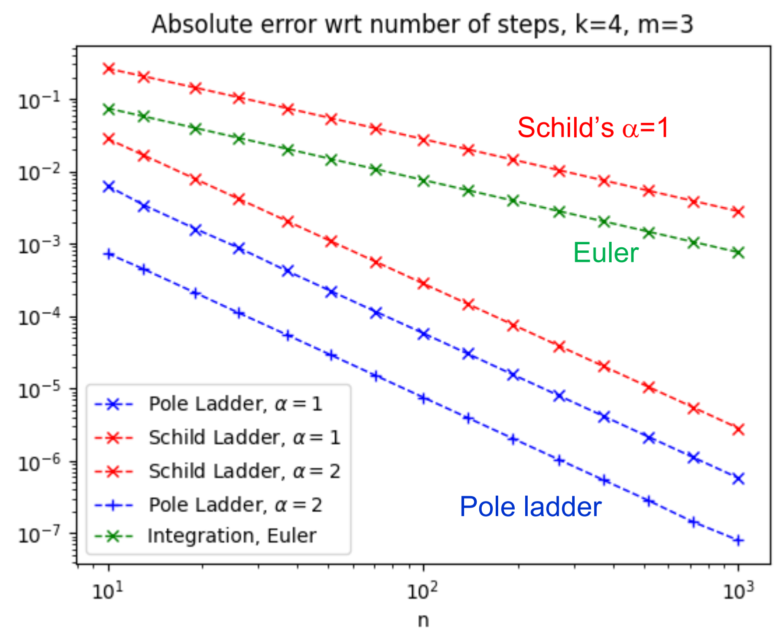


Numerical experiments in controlled spaces

Anisotropic metric on the Lie group SE(3)



Kendall shape space Σ_3^3



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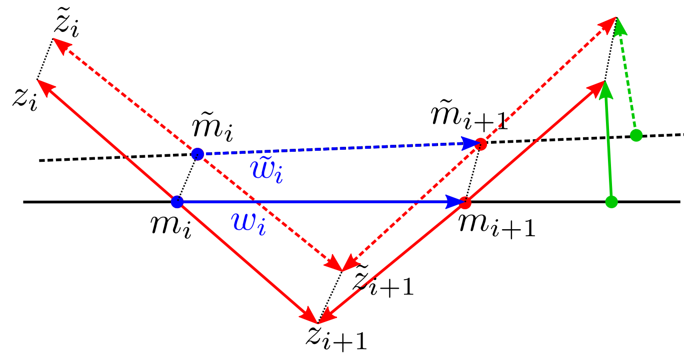
Approximate geodesics & other schemes

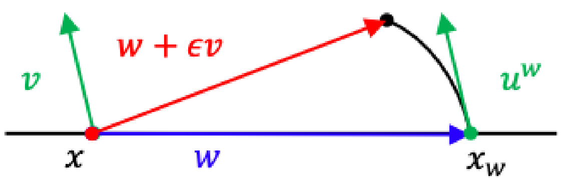


Approximated geodesics

- Integration using Runge-Kutta
- Compute the log by gradient descent

- Convergence results remain valid with sufficiently accurate numerical scheme

Fanning Scheme [Louis et al 2018]



$$\frac{u}{h\epsilon} = v + \frac{h^2}{6} R(w, v) w + O(h^3).$$

- Can be analyzed similarly
- Cannot ne made 2nd order

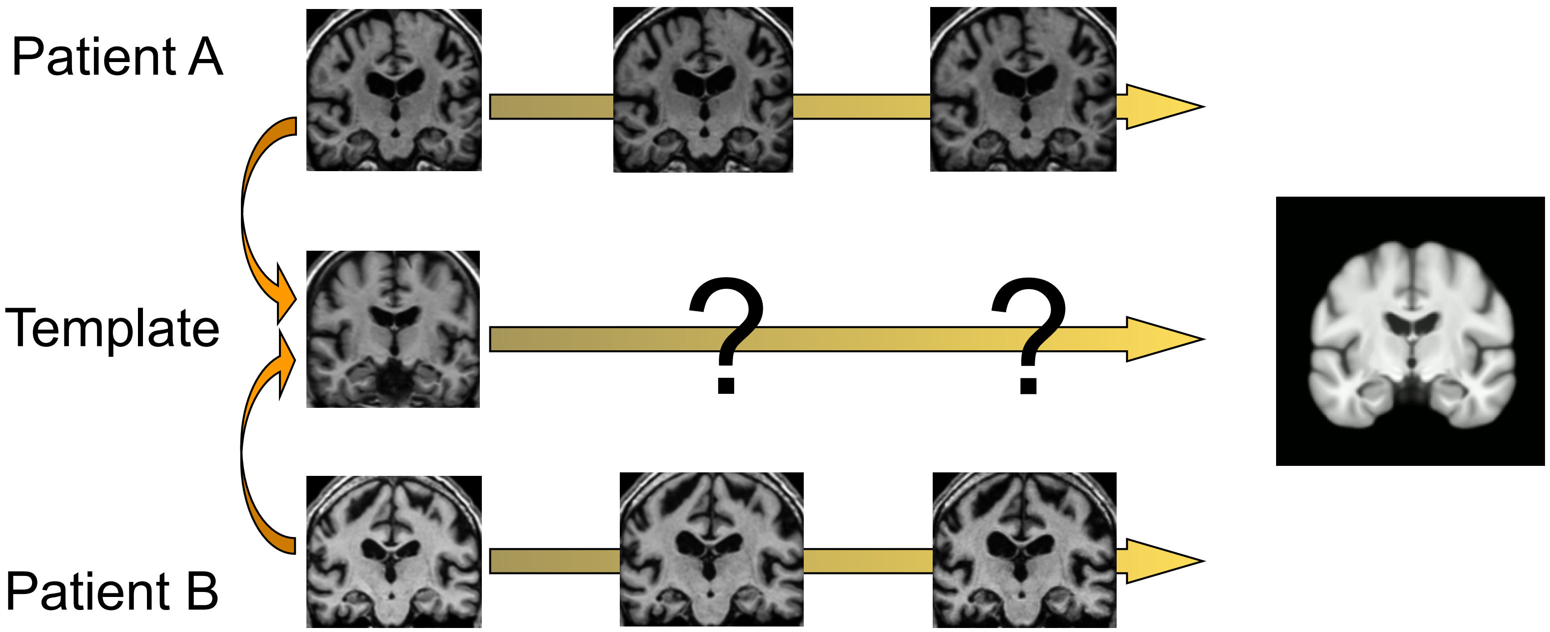
$$\|v_n - \Pi_x^{x_n} v\| \leq \frac{\beta}{n}.$$

[N. Guigui, XP, Numerical Accuracy of Ladder Schemes for Parallel Transport on Manifolds. Foundations of Computational Mathematics, 22:757-790, 06-2022. Arxiv 2007.07585.]

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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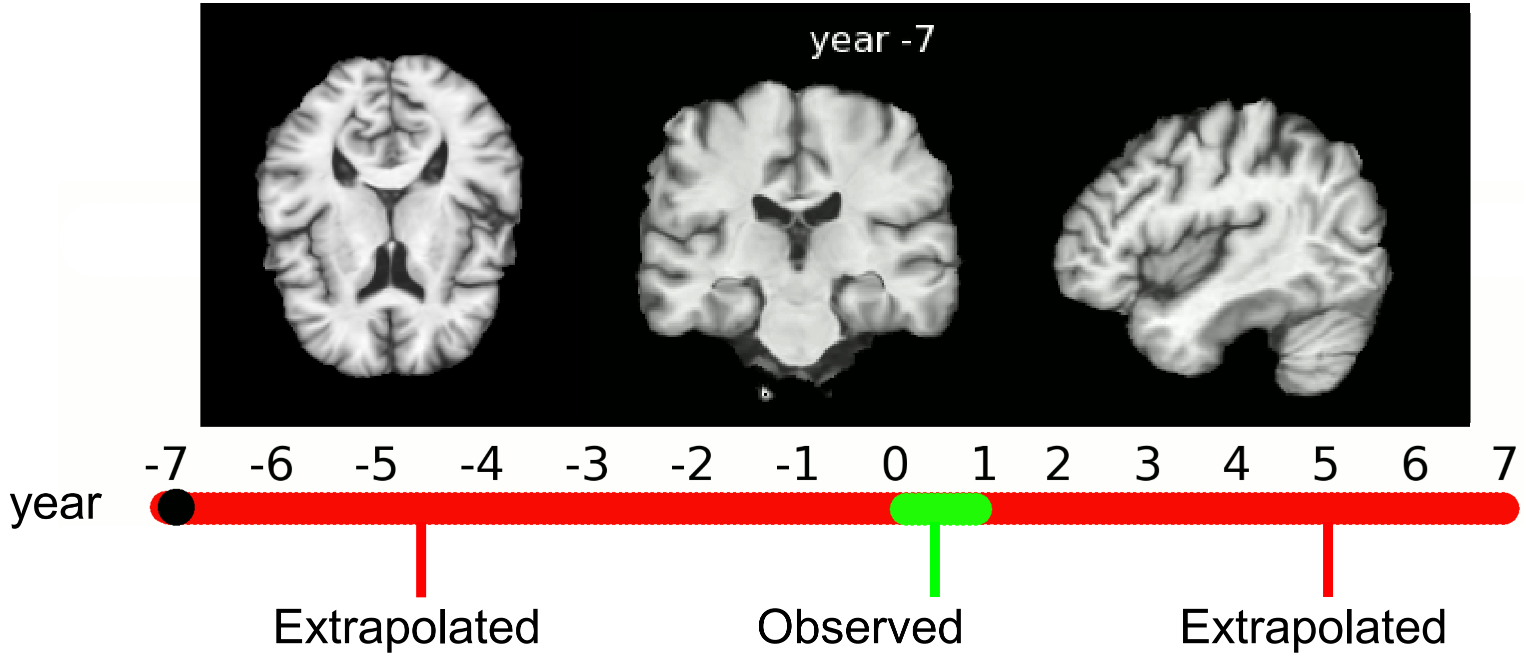
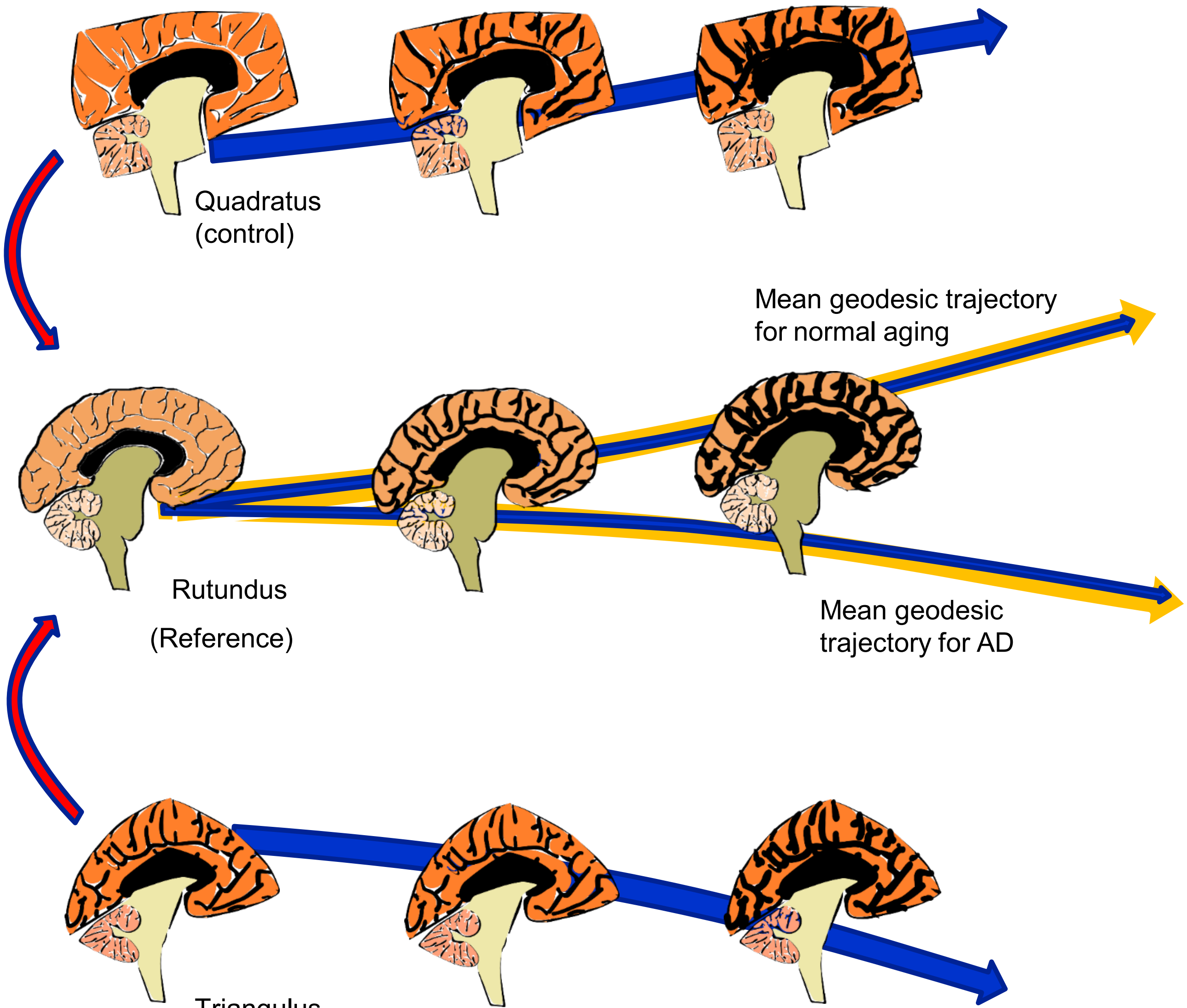
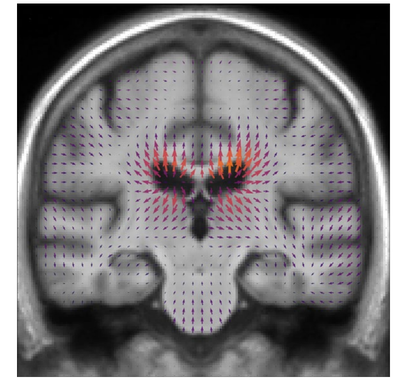


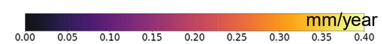
Modeling Normal and AD progression

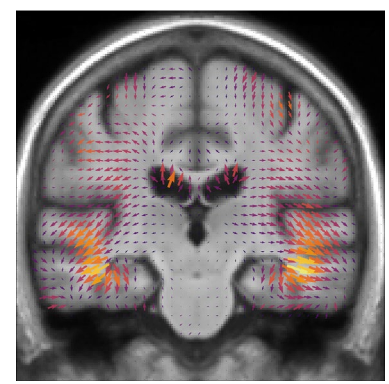


SVF parametrizing the deformation trajectory



Normal aging

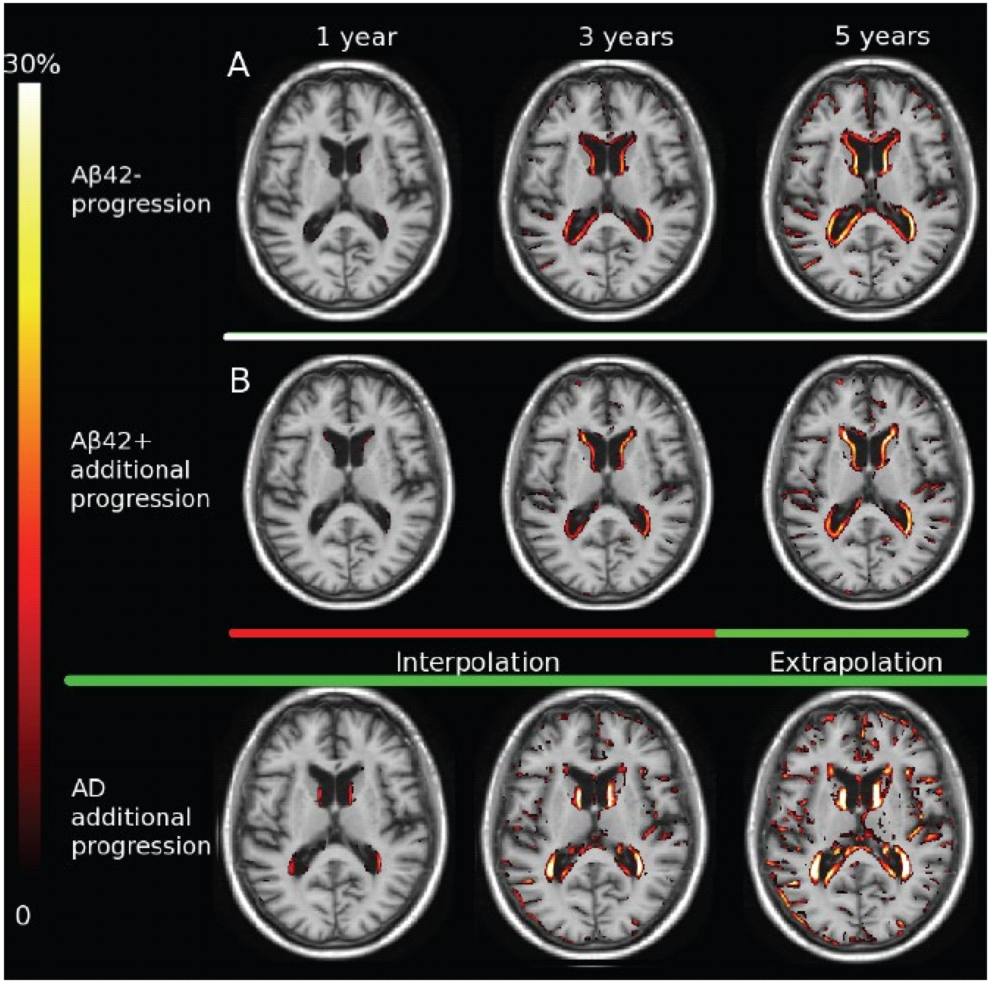




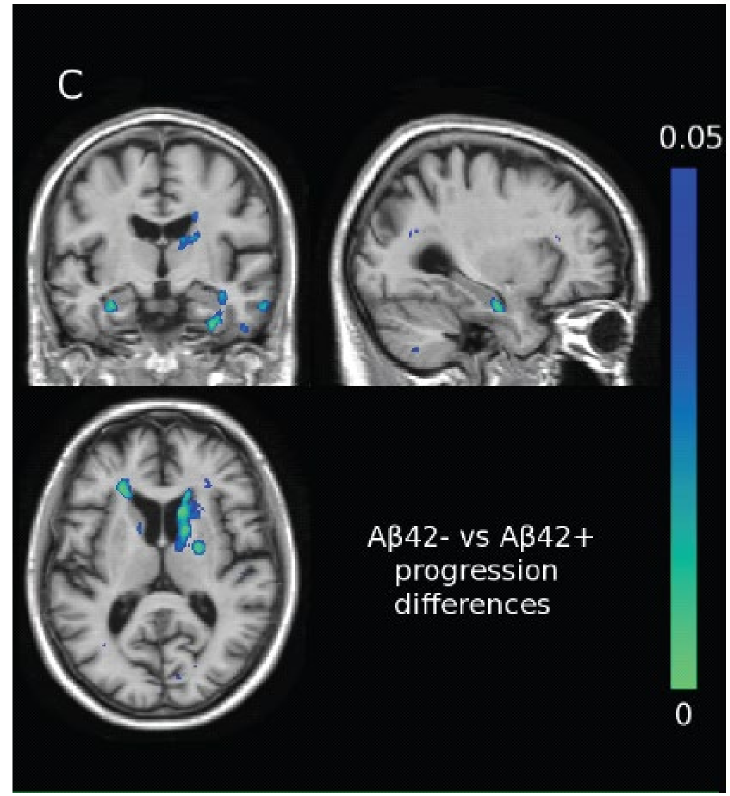
Addition specific component for AD

Study of prodromal Alzheimer's disease

Linear regression of the SVF over time: interpolation + prediction



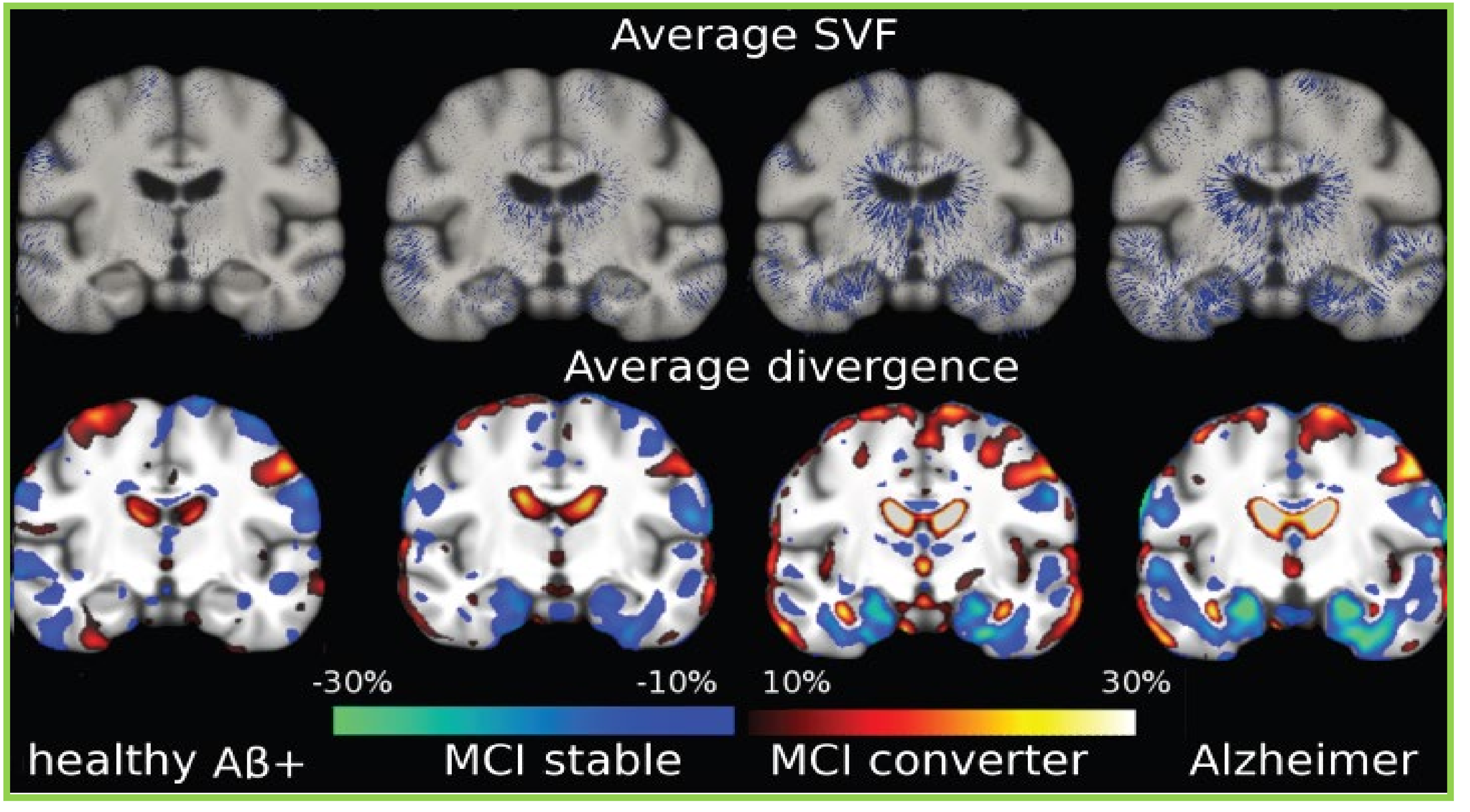
$$T(t) = Exp(\tilde{v}(t)) * T_0$$



Multivariate group-wise comparison of the transported SVFs shows statistically significant differences (nothing significant on log(det))

[Lorenzi, Ayache, Frisoni, Pennec, in Proc. of MICCAI 2011]

Mean deformation / atrophy per group



M Lorenzi, N Ayache, X Pennec G B. Frisoni, for ADNI. Disentangling the normal aging from the pathological Alzheimer's disease progression on structural MR images. 5th Clinical Trials in Alzheimer's Disease (CTAD'12), Monte Carlo, October 2012. (see also MICCAI 2012)

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- XP, M. Lorenzi. **Beyond Riemannian Geometry - The affine connection setting for transformation groups**. *In Riemannian Geometric Statistics in Medical Image Analysis*, Chap. 5, pp.169-229 RGSMIA. Elsevier, 2020. [DOI: 10.1016/B978-0-12-814725-2.00012-1] [Preprint] .
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