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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

Geometric Statistics workshop 09/2019

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## 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

Advances Statistics: CLT \& PCA

## Natural Riemannian Metrics on Transformations

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

- Composition g o h and inversion $\mathrm{g}^{-1}$ are smooth
- Left and Right translation $L_{g}(f)=g \circ f \quad R_{g}(f)=f \circ g$
- Conjugation Conj $_{g}(f)=g \circ f \circ \mathrm{~g}^{-1}$
- Symmetry: $\mathrm{S}_{\mathrm{g}}(\mathrm{f})=\mathrm{g}$ of $\mathrm{f}^{-1}$ og

Natural Riemannian metric choices

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

Implementation

- Practical computations using left (or right) translations

$$
\operatorname{Exp}_{\mathrm{f}}(\mathrm{x})=\mathrm{f} \circ \operatorname{Exp}_{I d}\left(\mathrm{DL}_{\mathrm{f}^{(-1)}} \cdot \mathrm{x}\right) \quad \overrightarrow{\mathrm{fg}}=\log _{\mathrm{f}}(\mathrm{~g})=\mathrm{DL}_{\mathrm{f}} \cdot \log _{\mathrm{Id}}\left(\mathrm{f}^{(-1)} \circ \mathrm{g}\right)
$$

## General Non-Compact and Non-Commutative case

No Bi-invariant Mean for 2D Rigid Body Transformations

- Metric at Identity: $\operatorname{dist}\left(\operatorname{Id},\left(\theta ; t_{1} ; t_{2}\right)\right)^{2}=\theta^{2}+t_{1}^{2}+t_{2}^{2}$

ㅁ $\quad T_{1}=\left(\frac{\pi}{4} ;-\frac{\sqrt{2}}{2} ; \frac{\sqrt{2}}{2}\right) \quad T_{2}=(0 ; \sqrt{2} ; 0) \quad T_{3}=\left(-\frac{\pi}{4} ;-\frac{\sqrt{2}}{2} ;-\frac{\sqrt{2}}{2}\right)$

- 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:
$\square$ 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

Lie groups with bi-invariant pseudo-metric

[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


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## Basics of Lie groups

Flow of a left invariant vector field $\tilde{X}=D L . x$ 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: $x \in \mathfrak{g} \rightarrow \operatorname{Exp}(x)=\gamma_{x}(1) \epsilon G$
- 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: $\nabla_{\dot{\gamma}} \dot{\gamma}=0$
- $2^{\text {nd }}$ order differential equation: Normal coordinate system
- Local exp and log maps, well defined in a convex neighborhood

[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 : $\mathrm{M}(\mathrm{t})=\mathrm{A} \exp (\mathrm{t} . \mathrm{V})$
- 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 $S_{\psi}(\phi)=\boldsymbol{\psi} \boldsymbol{\phi}^{-1} \psi$

- Matrix geodesic symmetry: $S_{A}(M(t))=A \exp (-t V) A^{-1} A=M(-t)$
[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

- $\sum_{i} \log _{x}\left(y_{i}\right)=0$ [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

$$
\Sigma=\int \log _{x}(y) \otimes \log _{x}(y) \mu(d y)
$$

- Matrix expression changes with basis


## Other statistical tools

- Mahalanobis distance, chi ${ }^{2}$ test
a-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 $\sum \log \left(x^{-1} \cdot y_{i}\right)=0$
- Algorithm: fixed point iteration (local convergence)

$$
x_{t+1}=x_{t} \circ \operatorname{Exp}\left(\frac{1}{n} \sum \log \left(x_{t}^{-1} \cdot y_{i}\right)\right)
$$

- Mean stable by left / right composition and inversion


## Matrix groups with no bi-invariant metric

- Heisenberg group: bi-invariant mean is unique (conj. ok for solvable)
- Rigid-body transformations: uniqueness if unique mean rotation
- $\operatorname{SU}(\mathrm{n})$ and $\mathrm{GL}(\mathrm{n})$ : 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

$$
T_{1}=\left(\frac{\pi}{4} ;-\frac{\sqrt{2}}{2} ; \frac{\sqrt{2}}{2}\right) \quad T_{2}=(0 ; \sqrt{2} ; 0) \quad T_{3}=\left(-\frac{\pi}{4} ;-\frac{\sqrt{2}}{2} ;-\frac{\sqrt{2}}{2}\right)
$$

$\square$ Metric at Identity: $\operatorname{dist}\left(\operatorname{Id},\left(\theta ; t_{1} ; t_{2}\right)\right)^{2}=\theta^{2}+t_{1}^{2}+t_{2}^{2}$

- 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 $\operatorname{Exp}_{x}$ 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?


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## Riemannian Metrics on diffeomorphisms

Space of deformations

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

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

Right invariant metric

- Eulerian scheme

$$
\left\|v_{t}\right\|_{\phi_{t}}=\left\|v_{t} \circ \phi_{t}^{-1}\right\|_{I d}
$$

- Sobolev Norm $H_{k}$ or $\mathrm{H}_{\infty}$ (RKHS) in LDDMM $\rightarrow$ diffeomorphisms [Miller, Trouve, Younes, Holm, Dupuis, Beg... 1998 - 2009]

Geodesics determined by optimization of a time-varying vector field

- Distance

$$
d^{2}\left(\phi_{0}, \phi_{1}\right)=\arg \min _{v_{t}}\left(\int_{0}^{1}\left\|v_{t}\right\|_{\phi_{t}}^{2} d t\right)
$$

- Geodesics characterized by initial velocity / momentum

ㅁ Optimization for images is quite tricky (and lenghty)

## 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 $\exp (v)=\exp (v / 2)$ o $\exp (v / 2)$
- Computing the Jacobian: $\operatorname{Dexp}(\mathrm{v})=\operatorname{Dexp}(\mathrm{v} / 2) \mathrm{o} \exp (\mathrm{v} / 2) . \operatorname{Dexp}(\mathrm{v} / 2)$
- Updating the deformation parameters: BCH formula [Bossa MICCAI 2007] $\exp (\boldsymbol{v}) \circ \exp (\varepsilon \boldsymbol{u})=\exp (\boldsymbol{v}+\varepsilon \boldsymbol{u}+[\boldsymbol{v}, \boldsymbol{\varepsilon} \boldsymbol{u}] / 2+[\boldsymbol{v},[\boldsymbol{v}, \boldsymbol{\varepsilon} \boldsymbol{u}]] / 12+\ldots)$
- Lie bracket $[\mathbf{v}, \boldsymbol{u}](\mathrm{p})=\operatorname{Jac}(\boldsymbol{v})(\mathrm{p}) . \boldsymbol{u}(\mathrm{p})-\operatorname{Jac}(\boldsymbol{u})(\mathrm{p}) . \boldsymbol{v}(\mathrm{p})$


## Parallel transport of deformation trajectories



## SVF setting

- v stationary velocity field
- Lie group Exp(v) non-metric geodesic wrt Cartan connections


## LDDMM setting

- v time-varying velocity field
- Riemannian $\exp _{i d}(v)$ metric geodesic wrt Levi-Civita connection
- Defined by intial momentum



## Transporting trajectories:

## Parallel transport of initial tangent vectors

LDDMM: parallel transport along geodesics using Jacobi fields [Younes et al. 2008]

## Parallel transport along arbitrary curves

A numerical scheme to integrate for symmetric connections:
Schild's Ladder [Elhers et al, 1972]

- Build geodesic parallelogrammoid
- Iterate along the curve

[ Lorenzi, Pennec: Efficient Parallel Transport of Deformations in Time Series of Images: from Schild's to pole Ladder, JMIV 50(1-2):5-17, 2013 ]


## Parallel transport along geodesics

Simpler scheme along geodesics: Pole Ladder
$\operatorname{Exp}(\Pi(u))=\operatorname{Exp}(v / 2) \circ \operatorname{Exp}(u) \circ \operatorname{Exp}(-v / 2)$
$\Pi_{B C H}(u)=u+[v, u]+\frac{1}{2}[v[v, u]]$

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## Parallel transport along geodesics

Simpler scheme along geodesics: Pole Ladder

Pole ladder is exact in 1 step in symmetric space


- Symmetry preserves geodesics:

$$
S_{m}(\gamma(t))=\gamma^{\prime}(t)
$$

- Parallel transport is differential of symmetry

$$
\gamma^{\prime}(t)=\exp _{P_{1}}(-\Pi(u))
$$

[ XP. Parallel Transport with Pole Ladder: a Third Order Scheme in Affine Connection Spaces which is Exact in Affine Symmetric Spaces. Arxiv 1805.11436]

## Accuracy of pole ladder

## Gavrilov's double exponential series (2006):

$$
\begin{aligned}
h_{x}(v, u) & =\log _{x}\left(\Pi_{x}^{\exp _{x}(v)} u\right) \\
& =v+u+\frac{1}{6} R(u, v) v+\frac{1}{3} R(u, v) u+\frac{1}{24} \nabla_{v} R(u, v)(2 v+5 u)+\frac{1}{24} \nabla_{u} R(u, v)(v+2 u)+O(5)
\end{aligned}
$$



Find u' that satisfies:

$$
h_{M}\left(v,-u^{\prime}\right)+h_{M}(-v, u)=0
$$



$$
u^{\prime}=u+\frac{1}{12} \nabla_{v} R(u, v)(5 u-2 v)+\frac{1}{12} \nabla_{u} R(u, v)(v-2 u)+O(5)
$$

- Error term is of order 4 in general affine manifolds
- Error is even zero for symmetric spaces: pole ladder is exact in one step!
[ XP. Parallel Transport with Pole Ladder: a Third Order Scheme in Affine Connection Spaces which is Exact in Affine Symmetric Spaces. Arxiv 1805.11436]


## 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


## The Stationnary Velocity Fields (SVF) framework for diffeomorphisms

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


## Modeling longitudinal atrophy in AD from images



## Study of prodromal Alzheimer's disease

Linear regression of the SVF over time: interpolation + prediction


$$
T(t)=\operatorname{Exp}(\tilde{v}(t)) * T_{0}
$$



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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