Shape Analysis and Computational Anatomy: A Geometrical Perspective on the Statistical Analysis of Population of Manifolds

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Outline

Building a differentiable and riemannian setting on shape spaces

Normal coordinates for statistical analysis

Means and Atlases

Currents and Manifold Representation

Statistics and statistical models

Challenges

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Anatomical shapes

Few anatomical structures segmented in MRI



Sulcal Lines

Internal Structures

Fiber Bundles

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Various shape spaces: points, surfaces, pieces of submanifolds, grey-level images, tensor fields, etc.

Anatomical shapes

Few anatomical structures segmented in MRI



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Various shape spaces: points, surfaces, pieces of submanifolds, grey-level images, tensor fields, etc.

Trivial metric don't work

- Differentiable structure should be compatible with "smooth" transformation of a shape (e.g. geometrical transformation)
- ▶ Not true for the L² metric on image and "smooth" transformations

$$au o au \dot{f}(\mathbf{x}) \doteq f(\mathbf{x} + au)$$

• $\tau \rightarrow t \cdot f$ is not smooth (but $\tau \rightarrow \tau$ is !).

A global geometrical setting through Riemannian submersion from a group of transformation onto a homogeneous space

• Consider a transitive group action i.e.

$$egin{array}{ccc} G imes M &
ightarrow & M \ (g,m) &
ightarrow & g.m \end{array}$$

where $M = G\dot{m}_0$ with $m_0 \in M$ ("template").

▶ If G is equipped with a G₀ (isotropy group) equivariant metric then

 $d_M(m,m') = \inf\{ d_G(g,g') \mid g.m_0 = m, g'.m_0 = m'\}$

is a distance on M (coming from the projected riemannian distance on M)

$$G/G_0 \simeq M$$

Simple framework: Right invariant metric on G (standard construction on finite dimensional Lie group).

(Video) Example on the sphere (landmarks matching) (J. Glaunes) = ,

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Thm (T.)

For any $V \hookrightarrow C_0^1(\mathbb{R}^d, \mathbb{R}^d)$ there exists $G_V \subset \text{Diff}^1(\mathbb{R}^d)$ with a right invariant distance d_G for which

- ► *G_V* is complete
- There exists a minimizing geodesic between any two elements in G_V $d_G(\mathrm{Id}, \phi)^2 = \inf\{\int_0^1 |v_t|^2 dt \mid \dot{\phi} = v \circ \phi, \phi_1 = \phi\}$

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Common representation framework



Exponential mapping

$$\begin{array}{rccc} \exp_{m_0}: & T_{m_0}M & \to & M \\ & \delta m_0 & \to & \exp_{m_0}(\delta m_0) \end{array}$$

such that $t \to \exp_{m_0}(t \delta m_0)$ is the solution of the geodesic equation

 $\nabla_{\dot{m}}\dot{m}=0$

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starting from m_0 with initial velocity δm_0 .

► Local diffeomorphism (when dim*M* < ∞)</p>

Feasibility of the normal coordinate computation



Reduction via momentum map





- v = Kj(m, p) (Horizontal lift)
- Maximum Pontryagin Principle

$$H_r(m,p) = \max_v H(m,p,v)$$

Hamiltonian evolution:

$$\dot{m} = \frac{\partial H_r}{\partial p}$$

 $\dot{p} = -\frac{\partial H_r}{\partial q}$

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Reduction and statistical power

A geodesic on *M* comes from a geodesic on G but its initial velocities v₀ or its momentum Lv₀ belongs to a subspace

$$V_0^* = j(m_0, T_{m_0}^*M) \subset V^*$$

So, geodesic optimization \Rightarrow dimensionality reduction \Rightarrow better statistical power.

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Curve example: γ₀ : [0, 1] → ℝ^d a continuous curve. Then p₀ is a vectorial measure M_f([0, 1], ℝ^d) = C([0, 1], ℝ^d)* and

$$v_0(x) = \int_0^1 K(x,\gamma_0(s)) dp_0(s) \;\; K(x,y) \in \mathcal{M}_d(\mathbb{R})$$
 kernel

 Moreover, if the geodesic comes from a smooth inexact matching problem e.g.

$$g(\gamma_1) = \int |\gamma_{\sf obs} - \gamma_1(s)|^2 ds$$

then $p_1 + \frac{\partial g}{\partial \gamma}(\gamma_1) = 0$ and $p_1 \in C([0, 1], \mathbb{R}^d)$. Same is true for p_0

For images, if the template is smooth and the data attachment term is smooth e.g. g(l₁) = ∫ |l_{obs} − l₁|²(x)dx then

$$v_0(x) = \int K(x,y) p_0(y) \nabla I_0(y) dy$$

 $Lv_0 = p_0 \nabla I_0$ distribution of vector fields normal to the level set of I_0 .

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Karcher means

For a data set $\{m_i\}$ 1 $\leq i \leq n$ the *Karcher mean* is the point m_0 minimizing

$$V(m_0) \doteq \sum_{i=1}^n d_M(m_0, m_1)^2$$

► Existence and uniqueness for finite dimensional *M* and {*m_i*} sufficiently closed or under negative curvature condition. Situation unclear for dim*M* = ∞.



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• Usually observations are y_i belongs to an observation space \mathcal{Y} different from *M*. Need the introduction of a data attachment term.

$$\underset{m_{0},m_{1},\cdots,m_{n}}{\text{minimize}} \sum_{i=1}^{n} d_{M}(m_{0},m_{1})^{2} + \lambda \sum_{i=1}^{n} r(m_{i},y_{i})$$

or equivalently (lift on the group G)

$$\underset{m_{0},\phi_{1},\cdots,\phi_{n}}{\text{minimize}} \sum_{i=1} d_{G}(\mathsf{Id},\phi_{i})^{2} + \lambda \sum_{i=1}^{n} r(\phi_{i}.m_{i},y_{i})$$

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Hypertemplate setting

$$\underset{m_{0},\phi_{1},\cdots,\phi_{n}}{\text{minimize}} \sum_{i=1} d_{G}(\mathsf{Id},\phi_{i})^{2} + \lambda \sum_{i=1}^{n} r(\phi_{i}.m_{i},y_{i})$$

- ► Variational problem: if *r* is smooth enough we have existence of a solution *φ̂_i*, ..., *φ̂_n* for *m*₀ fixed: *n* pairwise matching problems.
- If m_0 is let free, existence issues if dim $(M) = +\infty$.
- ▶ Introduce an hypertemplate m_h and look for $m_0 = \psi . m_h$ solution of

$$\underset{\psi,\phi_1,\cdots,\phi_n}{\text{minimize}} d_G(\mathsf{Id},\psi)^2 + \sum_{i=1}^n d_G(\mathsf{Id},\phi_i)^2 + \lambda \sum_{i=1}^n r(\phi_i \circ \psi.m_h,y_i)$$

 $\hat{m}_0 = \hat{\psi}.m_h, \, \hat{m}_1 = \hat{\phi}_i.\hat{m}_0$ Actually used to build atlases in medical imaging

Means and Atlases

Atlas learning through hypertemplate



Figure: 3D hippocampuses data.- Ma, Miller, T., Younes Neuroimage'08

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Why using currents ?

- Challenging problem for submanifold data :
- if X is a submanifold, it does not depend as a manifold on any particular parametrization (up to smooth chart changes)
- Noisy observation of manifolds may not be a smooth manifold or a manifold at all !

What is a current ?

- Goes back to De Rham. Introduced in this setting by Glaunes and Vaillant.
- Currents integrate differential forms

$$\omega \in \underbrace{\Omega_0^p(\mathbb{R}^d)}_{X \to X} \to C_X(\omega) = \int_X \omega \in \mathbb{R}$$

cont. p-form

On a chart $\gamma: U \to X \subset \mathbb{R}^d$

$$\int_{\gamma(U)} \omega \doteq \int_{U} \omega_{\gamma(s)} (\frac{\partial \gamma}{\partial s_1} \wedge \dots \wedge \frac{\partial \gamma}{\partial s_p}) ds$$

but the expression in independent of a smooth positively oriented reparametrization of the coordinate space $\psi : U \rightarrow U$

$$\frac{\partial \gamma \circ \psi}{\partial s_1} \wedge \dots \wedge \frac{\partial \gamma \circ \psi}{\partial s_p} = \mathsf{Jac}(\psi)(\frac{\partial \gamma}{\partial s_1} \wedge \dots \wedge \frac{\partial \gamma}{\partial s_p}) \circ \psi$$

X can be seen as an element of (Ω^ρ₀(ℝ^d))*. Depends on the orientation of X (X is an orientable manifold).

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RKHS norms on currents

- Idea: if W is a RKHS on the space on p-forms and W → Ω^p₀(ℝ^d) then Ω^p₀(ℝ^d)^{*} → W^{*} (W dense subset of Ω^p₀(ℝ^d)). We get an hilbertian structure on currents (dual norm).
- A kernel for *p*-forms is given as K : ℝ^d × ℝ^d → (Λ^pℝ^d ⊗ Λ^pℝ^d)^{*} and if X, Y are two orientable sub-manifolds

$$\langle \mathcal{C}_X, X_Y \rangle_{W^*} \doteq \int_{X \times Y} \mathcal{K}$$

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Punctual currents and approximations

► $\xi \in \Lambda^{p} \mathbb{R}^{d}$, $x \in \mathbb{R}^{d}$ define a punctual current $\xi \otimes \delta_{x} \in W^{*}$ such that

 $(\xi \otimes \delta_{\mathbf{X}} | \omega) = \omega_{\mathbf{X}}(\xi)$



• Discretization : line
$$\gamma : [0, 1] \rightarrow \mathbb{R}^d$$

$$\mathcal{C}_{\gamma}\simeq\sum_{i=1}^n(\gamma(\pmb{s}_{i+1}-\pmb{s}_i))\otimes\delta_{(\gamma(\pmb{s}_i)+\gamma(\pmb{s}_{i+1})/2}$$

Triangulated surface :

 $T(a, b, c) \rightarrow \xi \otimes \delta_x$

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with x = (a + b + c)/3 and $\xi = \vec{ab} \wedge \vec{ac}$.

 Make sense for arbitrary dimensions p and d.

Matching pursuit algorithm

Start from an initial manifold and $C_0 = C_X$ and iterate :

$$(x_{n+1}, \xi_{n+1}) = \operatorname{argmax}_{x,\xi} \langle \xi \otimes \delta_x, \underbrace{C_X - C_n}_{\text{residual}} \rangle_{W^*}$$
$$C_{n+1} = C_n + \xi_{n+1} \otimes \delta_{x_{n+1}}$$

- Very convenient to get compressed representation of manifolds
- Complexity control via sparse non parametric approximations

-Durrleman, Pennec, T., Ayache MICCAI'08.

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Currents and means (Atlas construction for manifolds)

1. Define a *parametrization invariant* data attachment term: for *X* and *Y* two orientable submanifold (same dimension)

$$r(X, Y) = h(|C_X - C_Y|_{W^*}).$$

2. Easy to consider noisy observation as currents $\mathcal{Y} = W^*$ and to defined generalized Karcher means :

minimize
$$\sum_{C_0,\phi_1,\cdots,\phi_n} \sum_{i=1}^n d_G (\mathrm{Id},\phi_i)^2 + \lambda \sum_{i=1}^n |\phi_i.C_0 - y_i|_{W^*}^2$$

where $(\phi, C) \rightarrow C.\phi$ is the push forward action.

3. For ϕ_1, \dots, ϕ_n fixed feasible computation of C_0 even with a large number of observations y_i (control of the number of points via matching pursuit).

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Atlas construction for fiber tracts



Figure: 5 fiber tracts segmented in 6 subjects

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Currents and Manifold Representation

Atlas construction for fiber tracts



Figure: Computed Template - Durrleman, Fillard, Pennec, T., Ayache Neuroimage'11

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Deformation analysis

- ▶ \$\hftau_1, \dots, \hftau_n\$ gives initial momentum \$\hftau_1, \dots, \hftau_n\$ the statistical analysis in the (finite dimensional) tangent space.
- PCA analysis (using the induced metric)

The analysis can be lifted on the space of diffeomorphism by horizontal lift giving generative model via shooting.

Sulcal lines: pairwise registration first mode



Deformation + textures (for manifolds)

Deformations

$$\hat{\phi}_1, \cdots, \hat{\phi}_n \longrightarrow \hat{p}_1, \cdots, \hat{p}_n$$
.

Texture : Residues

$$\hat{R}_i = y_i - \hat{\phi}. C_0 \in W^*$$

Analysis of the joint model

Fiber tracts: Deformation pairwise registration first mode (corticobulbar tract)



Deformation + textures (for manifolds)

Deformations

$$\hat{\phi}_1, \cdots, \hat{\phi}_n \longrightarrow \hat{p}_1, \cdots, \hat{p}_n.$$

Texture : Residues

$$\hat{R}_i = y_i - \hat{\phi}. C_0 \in W^*$$

Analysis of the joint model

Fiber tracts: First Mode of Residues (corticobulbar tract)

texture mode at $-\sigma$ $\bar{B} - m_{\varepsilon}$

texture mode at $+\sigma$ $\bar{B} + m_{\varepsilon}$

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Discrimination study workflow

- Learning of a common template + analysis in normal coordinates
- Application there of stander classification/discrimination methods
- Analysis of log(Jac(Φ)) on the template (atrophy patterns).

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Population analysis via bayesian mixed-effects hierarchical model

 $\mathbf{y}_i = \phi_i \cdot (\mathbf{m}_0 + \mathbf{T}_i) + \sigma \mathbf{n}_i$

- Fixed effects (population effects): template m₀, law of the deformations φ, law of the texture model T, noise level σ: θ = (m₀, p_φ, p_T, σ).
- ▶ Random effects (individual effects): individual deformation ϕ_i , texture T_i .
- Many hidden-variables: ϕ_i 's, T_i 's, n_i 's.
- ► Hyperparameters: priors on the fixed effect distribution.

$$\hat{\theta} = \operatorname*{argmax}_{\theta} P(\theta | y_1, \cdots, y_n)$$

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Deterministic algorithm as approximations of stochastic ones

 $\mathbf{y}_i = \phi_i (\mathbf{m}_0 + \mathbf{T}_i) + \sigma \mathbf{n}_i$

- Usual deterministic method for atlas learning appear to be straightforward approximations of EM-type algorithms (where the E-step is replaced by the mode approximation of the posterior distribution on the hidden variables)- Allassonnière, Amit, T. JRSS'07
- We could use this statistical setting to propose better algorithms: MCMC methods for the posterior distribution. -Kuhn and Lavielle, Compt. Stat. and Datata Analysis'05, Allassonniere, Kuhn, T. Bernoulli'10

Current state-of-the-art: Finite dimensional setting pour the fixed effects, no texture, SAEM-MCMC algorithms, linear deformation model, images.

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Templates estimation through SAEM-MCMC algorithm





Estimated templates

Simulated estimated deformation law

 Figure: US-Postal database, from Allassonnière et al., Bernoulli'10. Single model,

 SAEM-MCMC algorithm

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Templates estimation through SAEM-MCMC algorithm



Figure: US-Postal database, from Allassonnière et al., Bernoulli'10. Robustness to noise: Mode approximation Versus SAEM-MCMC algorithm

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Mixture models

Statistical models extended to mixture models allowing multi-template estimation



Figure: US Postal database - multi-template learning via mixture model. From Allassonniere, Kuhn ESAIM P&S'10

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- Proper statistical modeling and model estimation point of view appears to be a promising avenue in this high dimensional setting compared to more purely model free deterministic point of view
- In particular, integration of the posterior distribution of deformations instead of mode approximation is necessary for consistent model estimation and to work in noisy situations.

- However, still a high computational burden for MCMC sampling since the hidden variable are living in a high dimensional space. This implies the need of better adapted sampling scheme using the implicit low dimensionality of the high posterior log-likelihood curved submanifold (*Riemannian Manifold Hamiltonian Monte Carlo*, Girolami, Calderhead, Chin JRSS'10).
- Extension to the non linear situation using momentum representation and geodesic shooting is possible (work in progress)
- Manifolds: extension to the manifold setting is not done yet. Nor the estimation in this framework of a texture part (fiber tracks).
- Current implementation and theoretical work for the statistical modeling is restricted to the finite dimensional setting. Needs to understand the limit to the infinite dimensional setting.

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Next frontier: Modeling shape evolution and growth

An emerging question

- An emerging question of interest is now to study the time dependent data of shapes (images, landmarks, surfaces or tensors).
- Main target application: Growth studies, longitudinal studies.

with specific needs and challenges

- Flexibility: more or less non parametric models
- Versatility (various data and contexts)
- Robustness (noise, time sampling)
- Interpretability (ideally generative stochastic models)

	time			
0	0	\bigcirc	\bigcirc	
subjects				
	Δ	Δ_{i}	$ \land $	

Piecewise Geodesics Models



Miller's Growth Model (TS-LDDMM)

$$\hat{\mathbf{x}}_t = \phi_t \cdot \mathbf{x}_0, \ (\partial_t \phi = \mathbf{v}_t \circ \phi)$$
$$\inf_{\mathbf{v}} \int_0^1 |\mathbf{v}_t|^2 dt + \sum_{k=1}^n g_k(\phi_t \cdot \mathbf{x}_0, \mathbf{x}_{t_k}^{\text{obs}})$$

where $\mathbf{x}_{t_{\nu}}^{\text{obs}}$ are observed shapes (one subject).

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Piecewise Geodesics Models



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Piecewise Geodesics Models



Figure: Longitudinal growth model results for Huntington's Disease examining the caudate nucleus, From A. Khan and M. F. Beg, ISBI 2008.

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where $\mathbf{x}_{t_{\nu}}^{\text{obs}}$ are observed shapes (one subject).

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2nd order model: Shape Spline V Piecewise Geodesic



A few references

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