Optimal Riemannian quantization for air traffic management

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Context

Air traffic control

- Air traffic ontrollers act on flying or taxiing aircraft in such a way that separation norms are satisfied at all time.
- The airspace is segmented in elementary cells that can be regrouped or degrouped according to traffic complexity.
- Major concern : automatically evaluate the complexity of an air traffic situation.

What is an air traffic situation?

A set of positions and speeds (x_i, v_i) ∈ ℝ² × ℝ², i = 1,...,N of the aircraft present in the airspace at a given time.



A geometric complexity indicator

- In the neighborhood of each point (x_i, v_i), we assume that the spatial distribution of the speeds is Gaussian.
- We estimate its mean and covariance matrix using a kernel K, $K_h(x) = \frac{1}{h}K(\frac{x}{h})$,

$$m_i = \frac{\sum_{j=1}^N v_j K_h(x_i - x_j)}{\sum_{j=1}^N K_h(x_i - x_j)}, \quad \Sigma_i = \frac{\sum_{j=1}^N (v_j - m_i)(v_j - m_i)^T K_h(x_i - x_j)}{\sum_{j=1}^N K_h(x_i - x_j)}$$

- Σ_i measures the "local disorder" = "local complexity" of the traffic at point x_i
- We neglect the mean and represent complexity at x_i by $\mathcal{N}(0, \Sigma_i)$



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Information geometry

- Geometric approach to probability and statistics based on the Fisher information
- The Fisher information is defined for a parametric statistical model $\{p_{\theta}\mu|\theta\in\Theta\}$

$$I(\theta) = \mathbb{E}_{\theta}[\partial_{\theta}\ell_{\theta}(X) \cdot \partial_{\theta}\ell_{\theta}(X)^{t}], \quad \ell_{\theta} = \log p_{\theta}.$$

 In parametric estimation, the Fisher information gives a limit to the precision of the estimation given by an unbiased estimator T of θ function of a sample of size n (Cramer-Rao bound)

$$\operatorname{Var}_{\mathbf{\theta}}(T) \ge (nI(\mathbf{\theta}))^{-1}$$

• The Fisher information is the curvature of the Kullback-Leibler divergence $K(p,q) = \mathbb{E}_p \log(p/q)$

$$\partial_{\theta} K(\theta^*, \theta)|_{\theta=\theta^*} = 0, \quad \partial_{\theta_i} \partial_{\theta_j} K(\theta^*, \theta)|_{\theta=\theta^*} = I(\theta^*)_{i,j}$$

• The KL divergence is not symmetric and does not verify the triangular inequality. We use the Fisher information to define a real distance.

The Fisher information metric

• Parametric statistical model $\mathcal{P} = \{P_{\theta} = p_{\theta}\mu | \theta \in \Theta\}$ on \mathcal{X} , with $\Theta \subset \mathbb{R}^d$ open.

 Θ is a differentiable manifold, and can be equipped with a Riemannian metric using the Fisher information I(θ)

$$g_{\theta}(u,v) = u^t I(\theta) v, \quad u,v \in T_{\theta} \Theta \simeq \mathbb{R}^d$$

g is called the Fisher information metric or Fisher-Rao metric. (Θ,g) is a Riemannian manifold.

• The geodesic distance induced on Θ and therefore on $\mathcal P$

$$d_F(P_{\theta}, P_{\theta'}) = d_{\Theta}(\theta, \theta') = \inf_{\gamma, \gamma(0) = \theta, \gamma(1) = \theta'} \int_0^1 \sqrt{g_{\gamma(t)}(\dot{\gamma}(t), \dot{\gamma}(t))} dt,$$

is called the Fisher information distance.

Invariance properties of the Fisher information metric

• The Fisher geometry is invariant with respect to diffeomorphic parameter change $\forall \phi : \Theta \rightarrow \tilde{\Theta}, \theta \mapsto \tilde{\theta}$ diffeomorphism,

$$d_{\Theta}(\theta, \theta') = d_{\tilde{\Theta}}(\varphi(\theta), \varphi(\theta'))$$

 \rightarrow the geometric structure does not depend on the parameter choice.

• The Fisher metric is the only invariant metric with respect to sufficient statistics (Chentsov's theorem) : $T : X^n \to \mathbb{R}^d$ sufficient statistic of \mathcal{P} , i.e.

 $P_{\theta}((X_1,\ldots,X_n)|T(X_1,\ldots,X_n))$ is independent of θ

T transforms the sampling model $({P_{\theta}^n}_{\theta})_{\theta \in \Theta}, d_F^n)$ on \mathcal{X} into an isometric sampling model $({T_*(P_{\theta}^n)}_{\theta \in \Theta}, d_F^n)$ on \mathbb{R}^d

$$d_F^n(P_{\theta}^n, P_{\theta'}^n) = d_F^n(T_*(P_{\theta}^n), T_*(P_{\theta'}^n))$$

 \rightarrow the geometry of a parametric model is preserved through transformation by a sufficient statistic.

 $X \sim \mathcal{N}(m, \sigma^2)$ has probability density function

$$p_{\theta}(x) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(x-m)^2}{2\sigma^2}}, \qquad \theta = (m,\sigma) \in \mathbb{R} \times \mathbb{R}^*_+, \quad x \in \mathbb{R}.$$

The Fisher information is



The change of variables $(m, \sigma) \mapsto (m/\sqrt{2}, \sigma)$ yields the Poincaré half-plane, i.e. hyperbolic

The Wasserstein distance yields Euclidean geometry

$$\|d\theta\|^2 = dm^2 + d\sigma^2.$$

The geodesics yield optimal interpolations between probability distributions.



Since the curvature is negative, the Riemannian center of mass is well defined.



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Example : centered multivariate normal distributions

 $X \sim \mathcal{N}(0, \Sigma), \theta = \Sigma \in S_n^+$ symmetric positive definite matrix. The tangent vectors U, V in Σ are symmetric matrices

$$g_{\Sigma}(U,V) = \operatorname{tr}(\Sigma^{-1}U\Sigma^{-1}V).$$

The geodesics and geodesic distance have closed forms

$$\begin{split} \Gamma(t) &= \Sigma^{1/2} \exp\left(t\Sigma^{-1/2}U\Sigma^{-1/2}\right)\Sigma^{1/2}, \quad U \in T_{\Sigma}S_n^+ \\ d(\Sigma_1, \Sigma_2) &= \sqrt{\sum_{i=1}^n \log \lambda_i \left(\Sigma_1^{-1/2}\Sigma_2\Sigma_1^{-1/2}\right)}, \quad \lambda_i(A) = i^{\text{th}} \text{ eigenvalue of } A. \end{split}$$

This distance on S_n^+ is also called affine-invariant for its invariance w.r.t. GL_n

$$d(A^T \Sigma_1 A, A^T \Sigma_2 A) = d(\Sigma_1, \Sigma_2).$$

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- Goal : approximate $X \sim \mu$ by a quantized version q(X) where

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• Optimal quantization is an optimal transport problem (Graf, Luschgy, 2000)

$$\inf_{q\in Q_n} \mathbb{E}_{\mu}[d(X,q(X))^p] = \inf_{\nu\in \mathcal{P}_n(M)} W_p(\mu,\nu)^p,$$

where $\mathcal{P}_n(M) = \{v \text{ measure on } M, |\text{supp } v| \leq n\}$ and W_p is the p^{th} order Wasserstein distance, i.e.,

$$W_p(\mu, \mathbf{v}) = \inf_{P \in \Pi(\mu, \mathbf{v})} \int_{M \times M} d(y, z)^p dP(y, z),$$

where $\Pi(\mu, \nu) = \{ P \in \mathcal{P}(M \times M) \text{ has marginals } \mu \text{ and } \nu \}.$

Optimal quantization II

 The search for an optimal quantizer *q* can be restricted to nearest neighbor projections in a set α = {a₁,...,a_n} of size n

$$\begin{split} \inf_{q \in \mathcal{Q}_n} \mathbb{E}_{\mu} \left[d(X, q(X))^p \right] &= \inf_{\alpha = \{a_1, \dots, a_n\}} \mathbb{E}_{\mu} \left[d(X, q_{\alpha}(X))^p \right], \\ q_{\alpha}(x) &= \sum_{i=1}^n a_i \mathbf{1}_{Vi}(x), \quad x \in M, \\ V_i &= \{x \in M, d(x, a_i) \leq d(x, a_j) \, \forall j \neq i\} \quad \text{Voronoi cell.} \end{split}$$

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• The optimal quantization problem is written

$$\inf_{q\in Q_n} \mathbb{E}_{\mu}[d(X,q(X))^p] = \inf_{\alpha = \{a_1,\dots,a_n\}} \mathbb{E}_{\mu}\left[\min_{1\leq i\leq n} d(X,a_i)^p\right] = \inf_{\hat{\mu}\in P_n} W_p(\mu,\hat{\mu})^p,$$

where

$$Q_n = \{q : M \to M \text{ measurable}, |q(M)| \le n\},\$$

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• The minimizers $q = q_{\alpha}, \alpha = \{a_1, \dots, a_n\}$ and $\hat{\mu}$ are related by :

$$\hat{\mu} = (q_{\alpha})_* \mu = \sum_{i=1}^n \mu(V_i) \delta_{a_i}.$$

Finding the optimal quantized measure I

• We choose to optimize over n-tuples $\alpha = \{a_1, \dots, a_n\}$. We set

$$F_{n,p}(a_1,\ldots,a_n) = \mathbb{E}_{\mu}\left[\min_{1\leq i\leq n} d(X,a_i)^p\right] = \int_M \min_{1\leq i\leq n} d(x,a_i)^p d\mu(x).$$

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• For n = 1, p = 2, optimal quantization is equivalent to approximating μ by its Riemannian center of mass

$$\bar{x} = \mathbb{E}_{\mu}(X) = \operatorname*{argmin}_{a \in M} \int_{M} d(x, a)^{2} d\mu(x).$$

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 Existence of a solution (LB, Puechmorel, 2019) Let *M* be a complete Riemannian manifold and μ a probability distribution on *M* with compactly supported density. Then the cost function *F_{n,p}* is continuous and admits a minimizer.
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- The minimizer is in general not unique, e.g. in case of symmetries of μ.
- Gradient of the cost function (LB, Puechmorel, 2019) Let α = (a₁,..., a_n) ∈ Mⁿ be a *n*-tuple of pairwise distinct components. Then F_{n,2} is differentiable and its gradient in α is

$$\operatorname{grad}_{\alpha}F_{n,2} = \left(-2\int_{\mathring{V}_{i}}\overrightarrow{a_{i}x}\mu(\mathrm{d}x)\right)_{1\leq i\leq n} = -2\left(\mathbb{E}_{\mu}\mathbf{1}_{\{X\in\mathring{V}_{i}\}}\overrightarrow{a_{i}X}\right)_{1\leq i\leq n},\quad(1)$$

where $\overrightarrow{xy} := \log_x(y)$.

• The average opposite direction of the gradient is given by

$$\begin{bmatrix} \mathbf{1}_{\{X\in \mathring{V}_1\}} \stackrel{\longrightarrow}{a_1X} \\ \vdots \\ \mathbf{1}_{\{X\in \mathring{V}_n\}} \stackrel{\longrightarrow}{a_nX} \end{bmatrix}$$

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- In practice : we know μ through i.i.d. realizations X_1, X_2, \ldots
- Algorithm (Competitive Learning Riemannian Quantization) Initialization : α(0) = (a₁(0),...,a_n(0)), discrete steps Σγ_k = ∞, Σγ²_k < ∞ For each new observation X_k, repeat until convergence :

1. find
$$i^* = \operatorname{argmin}_i d(X_k, a_i(k))$$
,

2. update

$$a_{i^*}(k+1) = \exp_{a_{i^*}(k)} \left(\gamma_k \overrightarrow{a_{i^*}(k)X_k} \right),$$
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• Theorem (LB, Puechmorel 2019, Bonnabel 2013) If the injectivity radius of M is uniformly bounded from below by I > 0, and if $(\alpha(k))_{k \ge 0}$ is computed using the above algorithm and a sample of a compactly supported distribution μ , then $F_{n,2}(\alpha(k))$ converges a.s. and $\operatorname{grad}_{\alpha(k)}F_{n,2} \to 0$ when $k \to \infty$ a.s.

Link with *k*-means clustering

• Let X_1, \ldots, X_N be an i.i.d. sample of empirical distribution

$$\mu = \frac{1}{N} \sum_{k=1}^{N} \delta_{X_k}$$

The associated optimal quantized distribution is

$$\hat{\mu}_n = \sum_{i=1}^n \frac{|V_i|}{N} \delta_{a_i},$$

where a_1, \ldots, a_n minimizes the sum of intra-class variance of each Voronoi cell

$$F_{n,2}(a_1,\ldots,a_n) = \sum_{i=1}^n \sum_{x_k \in V_i} d^2(x_k,a_i).$$

This is the cost function of the k-means algorithm. The clusters are given by the Voronoi cells.

Competitive Learning Quantization is an online version of the *k*-means algorithm
 → adapted to large datasets.

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geomstats

- Created by Nina Miolane and Xavier Pennec
- Python package that factorizes code for geometric statistics into a shared unit-test library, with several backends : numpy, tensorflow and pytorch.
- Riemannian geometry is implemented in geomstats.geometry with 4 base classes
 - Manifold and EmbeddedManifold
 - RiemannianMetric and InvariantMetric
- The other manifold classes inherit from these 4 base classes



Quantization in geomstats

- Machine Learning is implemented in geomstats.learning, using scikit-learn classes
 - BaseEstimator
 - ClassifierMixin, RegressorMixin, TransformMixin, ClusterMixin and others.

```
sphere = Hypersphere(dimension=2)
data = sphere.random_von_mises_fisher(kappa=10, n_samples=1000)
clustering = Quantization(metric=sphere.metric, n_clusters=4)
clustering = clustering.fit(data)
cluster_centers = clustering.cluster_centers_
labels = clustering.labels
```



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Real data analysis

• Given an air traffic image, we extract *N* SPD matrices $\Sigma_1, \ldots, \Sigma_N$, with empirical distribution $1 \sum_{k=1}^{N} s_k$

$$\mu = \frac{1}{N} \sum_{i=1}^{N} \delta_{\Sigma_i}$$

· We use optimal quantization to find a summary

$$\hat{\mu} = \sum_{i=1}^{n} w_i \delta_{A_i}$$
, where $w_i = |V_i|/N$.

- In practice, we choose n = 3 because the centers can then be ordered (Loewner order : A ≥ B ⇔ A − B positive definite).
- Mapping back the labels to the image, this yields a clustering of the image in zones of homogeneous complexity.



Three levels of complexity



Clustering of the airspace above Paris (left), Toulouse (middle) and Lyon (right).

Comparison to Euclidean geometry



Clustering of the French airspace with Fisher-Rao (up) vs Euclidean (down) geometry.

Comparison to human perception



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Comparison of summaries

To compare summaries $\mu = \mu_1 \delta_{A_1} + \mu_2 \delta_{A_2} + \mu_3 \delta_{A_3}$ and $\nu = \nu_1 \delta_{B_1} + \nu_1 \delta_{B_1} + \nu_1 \delta_{B_1}$, it suffices to find the transport plan $\pi = (\pi_{ij})_{i,j}$

π_{11}	π_{12}	π_{13}	μ
π_{21}	π_{22}	π_{23}	μ_{1}
π_{31}	π_{32}	π_{33}	μ_{2}

 $v_1 \quad v_2 \quad v_3$

solution of





Distances matrix between the summaries :

4.55	6.07	1.22	0.00	
6.74	8.31	0.00	1.22	
1.92	0.00	8.31	6.07	
0.00	1.92	6.74	4.55	

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Shape analysis

Some interesting questions :

- how can we compare two shapes?
- how can we interpolate between two shapes?
- how can we compute a mean shape?
- how can we perform clustering on shapes?



- \rightarrow Riemannian geometry : convenient framework to generalize
 - usual statistical notions (mean, covariance, Gaussian distribution...)
 - data processing algorithms (clustering, PCA...)

• We consider smooth curves in a space M (\mathbb{R}^n or manifold) with non zero speed

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$$\mathcal{M} = \{ c : [0,1] \to M \quad C^{\infty}, \quad c'(t) \neq 0 \; \forall t \}$$

- The space of curves ${\mathcal M}$ can be seen as an ($\infty\text{-dim})$ differentiable manifold



• We consider smooth curves in a space M (\mathbb{R}^n or manifold) with non zero speed

$$\mathcal{M} = \{ c : [0,1] \to M \quad C^{\infty}, \quad c'(t) \neq 0 \; \forall t \}$$

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$$G_c(v,w), \quad c \in \mathcal{M}, \quad v,w \in T_c \mathcal{M}, \quad \text{then}$$

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- ightarrow a geodesic in ${\mathcal M}$ is an interpolation between two curves
- \rightarrow dist $(c, c_1) = L$ (geodesic between $c \ge c_1$)

Model of a shape

· Curves are reparameterized by the action of increasing diffeomorphisms

 $c \mapsto c \circ \varphi, \qquad \varphi \in \Gamma := \mathsf{Diff}_+([0,1])$

• A shape is an element of the quotient space \mathcal{M}/Γ



• If the Riemannian metric on ${\mathcal M}$ is invariant w.r.t. the action of Γ

$$G_c(v,w) = G_{c \circ \varphi}(v \circ \varphi, w \circ \varphi), \quad \forall \varphi \in \Gamma$$

it induces a Riemannian metric on \mathcal{M}/Γ for which the distance is

$$\mathsf{dist}([c_0], [c_1]) = \inf_{\varphi \in \Gamma} \mathsf{dist}(c_0, c_1 \circ \varphi).$$

How to compare two shapes?

- To compare two shapes in \mathcal{M}/Γ :
 - 1. define a reparameterization invariant metric on ${\mathcal M}$
 - 2. find its geodesics (solve geodesic equations)
 - 3. solve the optimal matching problem φ between two curves c_0 et c_1

$$\mathsf{dist}([c_0], [c_1]) = \inf_{\varphi \in \Gamma} \mathsf{dist}(c_0, c_1 \circ \varphi)$$

• (Michor, Mumford, 2005) The reparameterization invariant *L*² metric yields a vanishing distance on the quotient space

$$G_c(w,z) = \int_0^1 \langle w(t), z(t) \rangle |c'(t)| dt$$

· Need to include higher order derivatives, e.g. elastic metrics

$$G_c^{a,b}(w,z) = \int a^2 \langle D_\ell w^N, D_\ell z^N \rangle + b^2 \langle D_\ell w^T, D_\ell z^T \rangle \, \mathrm{d}\ell$$

where $D_\ell w = w'/|c'|$, $d\ell = |c'(t)|dt$.



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The SRV framework

• For the special case a = 1, b = 1/2, the elastic metric can be mapped to an L^2 -metric through the square root velocity transform $q = c'/\sqrt{|c'|}$ (Srivastava et al. 2011)

$$d_{G^{1,\frac{1}{2}}}^{2}(c_{0},c_{2}) = d_{L^{2}}^{2}(q_{0},q_{1}) = \int_{0}^{1} |q_{1}(t) - q_{0}(t)|^{2} dt.$$



- Many extensions
 - curves in a manifold (J.Su et al. 2014, LB 2017, Zhang et al. 2018)
 - curves in a Lie group (Celledoni et al. 2016)
 - curves in homogeneous spaces (Z.Su et al. 2017, Celledoni et al. 2017)
 - surfaces (square root normal field, Jermyn et al. 2012)

Examples of geodesics between curves



Geodesics between curves in the Poincaré upper half-plane \mathbb{H}^2

Are we really comparing shapes?

• At this stage, the distance between two curves does not change if we reparameterize them the same way, but it does change if we reparameterize them in different ways !



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· We need to solve the optimal matching problem

$$\mathsf{dist}([c_0], [c_1]) = \inf_{\varphi \in \Gamma} \mathsf{dist}(c_0, c_1 \circ \varphi).$$

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Shape analysis framework Optimal matching

• Principal bundle structure $\pi: \mathcal{M} \to \mathcal{M}/\Gamma \Rightarrow$ Decomposition of the tangent space

 $T_c\mathcal{M}=V_c\mathcal{M}\oplus H_c\mathcal{M}$ Tangent vector = Vertical part + Horizontal part

- The vertical deformations are of the form w(t) = m(t)v(t) where v = c'/|c'|.
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- We decompose any path of curves $s\mapsto c(s,\cdot)\in \mathcal{M}$ into

$$c(s,t) = c^{hor}(s,\varphi(s,t)), \qquad \begin{array}{l} s \mapsto c^{hor}(s,\cdot) \text{ horizontal path} \\ s \mapsto \varphi(s,\cdot) \text{ path in Diff}^+([0,1]) \end{array}$$

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• Assuming that we know $\partial_s c(s,t)^{ver} = m(s,t)v(s,t)$, we can show (LB 2019) : The path of diffeomorphisms is solution of the PDE

$$\begin{cases} \partial_s \varphi(s,t) = \frac{m(s,t)}{|\partial_t c(s,t)|} \cdot \partial_t \varphi(s,t), \\ \varphi(0,t) = t. \end{cases}$$

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(LB 2019) For elastic metrics, the vertical part m(t) of a tangent vector w(t) verifies m(0) = m(1) = 0 and is solution of the ODE

$$m'' - \langle \nabla_t c' / |c'|, v \rangle m' - (a/b)^2 |\nabla_t v|^2 m$$

= $\langle \nabla_t \nabla_t w, v \rangle - ((a/b)^2 - 1) \langle \nabla_t w, \nabla_t v \rangle - \langle \nabla_t c' / |c'|, v \rangle \langle \nabla_t w, v \rangle.$

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 \rightarrow From a path of curves c(s,t), find m(s,t) for $w(s,t) = \partial_s c(s,t)$, then $\varphi(s,t)$ and then

$$c^{hor}(s,t) = c(s, \varphi(s)^{-1}(t))$$

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Sub-optimal matching



Optimal matching



Sub-optimal matching



Optimal matching



Sub-optimal matching



Optimal matching



Geodesics between curves vs between shapes



Real data applications

• Trajectory analysis



Comparison of hurricane tracks

Real data applications

• Mean shape of the internal ear (J. M. Loubes)



Thank you for your attention !