A Lower Bound for Estimating Fréchet Means In Memory of Laurent Cavalier († 2014)

CIRM Workshop: Geometric Sciences in Action: from Geometric Statistics to Shape Analysis at Luminy (May 27 - 31, 2024)

Stephan F. Huckemann
joint work with Benjamin Eltzner and **Shayan Hundrieser**

University of Göttingen,
Felix Bernstein Institute for Mathematical Statistics in the Biosciences

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Fréchet (1948) Means

Ingredients:

- metric space $(\mathfrak{X}, d)$, $\rho : \mathfrak{X} \times \mathfrak{X} \to \mathbb{R}$ continuous,
- Borel m'ble random variables $X_1, \ldots, X_n \overset{i.i.d.}{\sim} X \sim \mathbb{P}$ on $\mathfrak{X}$

$\rightsquigarrow$ Fréchet ρ-mean sets

$$\begin{aligned} \text{population} \quad \mathbb{M}(\mathbb{P}) &:= \operatorname{argmin}_{x \in \mathfrak{X}} \mathbb{E}[\rho(x, X)]\,, \\ \text{sample} \quad \mathbb{M}_n &:= \operatorname{argmin}_{x \in \mathfrak{X}} \frac{1}{n} \sum_{j=1}^{n} \rho(x, X_i)\,. \end{aligned}$$

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Existence for $\rho = d^2$:

- $\mathbb{M}_n \neq \emptyset$ a.s. if $(\mathfrak{X}, d)$ complete,
- $\mathbb{M}(\mathbb{P}) \neq \emptyset$ if additionally, $\exists x \in \mathfrak{X}$ with $\mathbb{E}[d(x, X)] < \infty$.

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Uniqueness:

- $|\,\mathbb{M}(\mathbb{P})| = 1$ if additionally $\operatorname{supp}(X)$ in ball, smaller than a goedesic half ball (Karcher, 1977; Kendall, 1990; Le, 2001; Groisser, 2005; Afsari, 2011).
- $|\,\mathbb{M}_n\,| = 1$ a.s. if additionally $\mathfrak{X}$ is a Riemannain manifold and X is absolutely continuous w.r.t. Riemannian volume (Arnaudon and Miclo, 2014).

Strong Law of Large Numbers

Kuratowski (1948) convergence of sets $C_n \subseteq \mathfrak{X}$, $n \in \mathbb{N}$:

$$\begin{aligned}
\underset{n\to\infty}{Ls}\, C_n &:= \{x \in Q : \liminf_{n\to\infty} d(x, C_n) = 0\} = \bigcap_{n=1}^{\infty} \overline{\bigcup_{k=n}^{\infty} C_k} \\
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Theorem (Ziezold (1977); Bhattacharya and Patrangenaru (2003))

If $\exists \in \mathfrak{X}$ *with* $\mathbb{E}[d(x, X)] < \infty$, $\mathfrak{X}$ *separable, then*

(ZC) $Ls_{n\to\infty} \mathbb{M}_n \subseteq \mathbb{M}(\mathbb{P})$ *a.s.,*

(BPC) *if* $\mathfrak{X}$ *is Heine-Borel and* $\mathbb{M}(\mathbb{P}) \neq \emptyset$ *then* $\mathbb{M}(\mathbb{P}) = Li_{n\to\infty} \mathbb{M}_n$ *a.s.*

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Extensions to generalized Fréchet means by H. (2011); e.g.

$$\text{argmin}_{\gamma\in\Gamma} \frac{1}{n}\sum_{j=1}^{n} d(\gamma, X_j)^2 \to \text{argmin}_{\gamma\in\Gamma} \mathbb{E}[d(\gamma, X)^2]$$

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Recent extensions by Schötz (2022); Wiechers et al. (2023); Evans and Jaffe (2024): (ZC) inclusion can be strict.

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   - that comes in different flavors (Lammers et al., 2023).
   - Can it be turned into a blessing?
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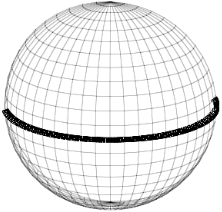
Nonuniqueness

Consider $x, y \in \mathfrak{X} = \mathbb{S}^2$ with

- $d_E(x, y) = \|x - y\|$ = extrinsic metric
- $d_I(x, y) = \arccos y^T x$ = intrinsic (spherical) metric
- $d_R(x, y) = \|x - yy^T x\|$ = residual quasi metric

and $X \sim$ uniform on equator:



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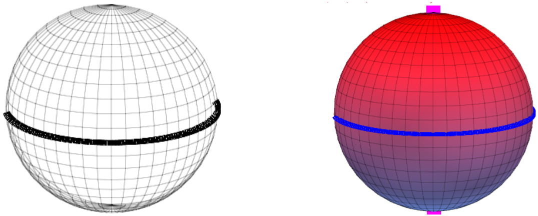

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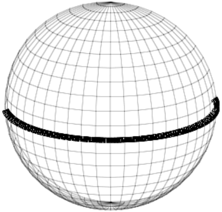

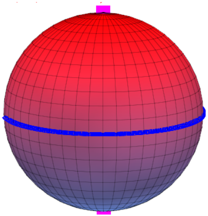

How, and how good is the estimation of random variables “near” X?

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Definition

A Fréchet ρ-mean $\mathbb{M}$ is honest if $\mathbb{M}(\delta_x) = \{x\}$ for all $x \in \mathfrak{X}$.

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Lemma 1 (Instability of Nonuniqueness)

For all honest $\mathbb{M}$ on $\mathfrak{X}$, all $t \in (0, 1]$ and all $x \in \mathbb{M}(\mathbb{P})$ we have

$$\mathbb{M}(\mathbb{P}_{x,t}) = \{x\}$$

with the perturbed measure $\mathbb{P}_{x,t} := (1 - t)\,\mathbb{P} + t\delta_x$.

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Fréchet d^2-means based on a metric d are honest, however, not if based on the residual quasi metric.

Lower Bound

Theorem 1

Let the Fréchet ρ-mean $\mathbb{M}$ be honest,

- $|\mathbb{M}(\mathbb{P})| > 1$,
- $n \in \mathbb{N}$ *fixed, whereas* $x \in \mathbb{M}(\mathbb{P})$, $0 < t \leq 1$ *arbitrary*
- $X_1, \ldots, X_n \overset{i.i.d.}{\sim} \mathbb{P}_{x,t}$,
- $\hat{\mu}_n$ *any estimator of* $\mathbb{M}$, *e.g.* $\hat{\mu}_n = \mathbb{M}_n$,

then for all $\eta > 0$,

$$\sup_{\substack{x \in \mathbb{M}(\mathbb{P}) \\ 0 < t \leq 1}} \mathbb{P}_{x,t}^{\otimes n} \left\{ d(\hat{\mu}_n, \mathbb{M}(\mathbb{P}_{x,t})) \geq \frac{\operatorname{diam} \mathbb{M}(\mathbb{P}) - \eta}{2} \right\} \geq \frac{1}{2} \,.$$

Proof

Apply argument chain of Tsybakov (2009, p. 79 ff.):

1. $y, z \in \mathbb{M}(\mathbb{P}), d(y, z) \geq \operatorname{diam}(\mathbb{M}(\mathbb{P}) - \eta,$

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   $\overset{(2.9),\ p.80}{\underset{\Delta\text{ ineq}}{\geq}} \quad \inf_{\psi_n} \max_{x \in \{y,z\}} \mathbb{P}_{x,t}^{\otimes n}\{\psi_n \neq x\} =: p_{e,1}$
   over all tests $\psi_n : \mathfrak{X}^n \to \{y,z\}$;
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6. $\overset{\text{p. 90,Thm 2.2 (i)}}{\Rightarrow} p_{e,1} \geq \frac{1-\alpha}{2}$,
7. $t \to 0 \Rightarrow \alpha \to 0 \Rightarrow$ Theorem 1 (max above $\leq$ sup of theorem).

Step 5: The Missing Inequality

Tsybakov (2009, p. 83, 86), two prob. distributions P, Q:

- squared Hellinger distance
  $$H(P,Q)^2 := \int \left(\sqrt{\frac{dP}{d\nu}} - \sqrt{\frac{dQ}{d\nu}} \right)^2 d\nu \text{ , } \nu = P + Q,$$
- total variation distance $TV(P,Q) := \sup_{A \text{ m'ble}} |P(A) - Q(A)|$,
- $H(P^{\otimes n}, Q^{\otimes n})^2 = 2\left(1 - \left(1 - \frac{H(P,Q)^2}{2}\right)^n\right)$,
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- $TV(\mathbb{P}_{y,t}^{\otimes n}, \mathbb{P}_{z,t}^{\otimes n})^2 \leq H(\mathbb{P}_{y,t}^{\otimes n}, \mathbb{P}_{z,t}^{\otimes n})^2 \leq 2\,(1 - (1-t)^n)$.

Remark 1

Given $\mathbb{M}(\mathbb{P}) \ni y \neq z \in \mathbb{M}(\mathbb{P})$, uniformly over

$$\{\mathbb{P}_{x,t} : x \in \{y, z\}, t \in (0, \epsilon)\}, \forall 0 < \epsilon \leq 1$$

no test $\psi_n \colon \mathfrak{X}^n \to \{y, z\}$ will perform better than a coin flip.

Corollary 1

Markov inequality $\frac{1}{2} \leq \mathbb{P}\{Y \geq s\} \leq \frac{\mathbb{E}[Y]}{s}$ and $\eta \to 0$ gives

$$\inf_{\hat{\mu}_n} \sup_{\substack{x \in \mathbb{M}(\mathbb{P}) \\ 0 < t \leq 1}} \mathbb{E}_{\mathbb{P}_{x,t}^{\otimes n}} [d(\hat{\mu}_n, \mathbb{M}(\mathbb{P}_{x,t}))] \geq \frac{\operatorname{diam} \mathbb{M}(\mathbb{P})}{4} .$$

Corollary 1

Markov inequality $\frac{1}{2} \leq \mathbb{P}\{Y \geq s\} \leq \frac{\mathbb{E}[Y]}{s}$ and $\eta \to 0$ gives

$$\inf_{\hat{\mu}_n} \sup_{\substack{x \in \mathbb{M}(\mathbb{P}) \\ 0 < t \leq 1}} \mathbb{E}_{\mathbb{P}_{x,t}^{\otimes n}} [d(\hat{\mu}_n, \mathbb{M}(\mathbb{P}_{x,t}))] \geq \frac{\operatorname{diam} \mathbb{M}(\mathbb{P})}{4} .$$

Example:

- $\mathbb{P} = \frac{\delta_N + \delta_S}{2}$ on $\mathbb{S}^2$ with poles N, S, resp.,
- d: spherical distance,
- $\mathbb{M}(\mathbb{P}) =$ equator, $\operatorname{diam} = \pi$,
- pick $x \in$ equator, zero meridian,
- as $t \to 0$ (by symmetry)
  - $\mathbb{M}_n$ of $\mathbb{P}_{x,t}^{\otimes n}$ tends to be on far side with 50 %,
  - in these cases $d(\mathbb{M}_n, x) \geq \pi/2$,
  - in the mean, $d(\mathbb{M}_n, x) \geq \pi/4$.

The Wasserstein World

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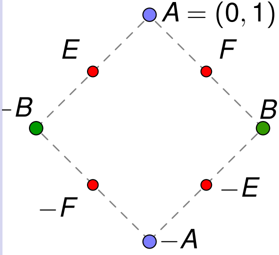
- $(\mathfrak{X}, d) := (\mathcal{P}_2(\mathbb{R}^m), \mathcal{W}) =$ the 2-Wasserstein space over $\mathbb{R}^m$,
- it's metric, hence its Fréchet means are honest.

Nonuniqueness in the Wasserstein World



In $\mathbb{R}^2$, let

$$\mu := \frac{1}{2}\left(\delta_A + \delta_{-A}\right),$$
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yielding,

$$\mathbb{M}(\mathbb{P}) = \left\{ \frac{\alpha}{2}(\delta_E + \delta_{-E}) + \frac{1-\alpha}{2}(\delta_F + \delta_{-F}) : 0 \le \alpha \le 1 \right\}.$$

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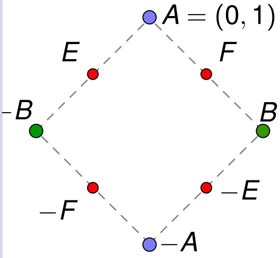

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By Corollary 1, for $\mathbb{M}_n$ of $\mu_1, \dots, \mu_n \overset{i.i.d.}{\sim} \mathbb{P}_{\mu,t} = (1-t)\,\mathbb{P} + t\delta_\mu$, $0 < t \le 1$ (by symmetry):

$$\sup_{t>0} \mathbb{E}_{\mathbb{P}_{\mu,t}^{\otimes n}}[\mathcal{W}(\mathbb{M}_n, \mu)] \ge \frac{\operatorname{diam} \mathbb{M}(\mathbb{P})}{4} = \frac{1}{4}\,,$$

as $\|F - E\| = 1 = \|F + E\|$.

Parametric Rates ($1/n$)

Theorem (Le Gouic et al. (2022), Cor. 1.2)

Let/assume:

- $0 < \alpha \leq \beta$, $\Phi_{\alpha,\beta} := \Big\{\phi \in \mathcal{C}^1(\mathbb{R}^m \to \mathbb{R}) :$
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Then, if $\beta < \alpha + 1$,

$$\mathbb{E}_{\mathbb{P}^{\otimes n}}[\mathcal{W}(\mathbb{M}_n, \tau)^2] \leq \frac{1}{n}\,\frac{4\,\mathbb{E}_{P\sim\mathbb{P}}[\mathcal{W}(P,\tau)^2]}{(\beta-\alpha-1)^2}\,.$$

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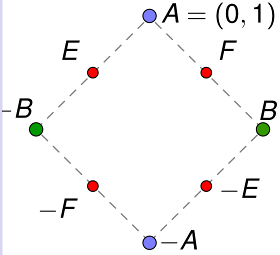
Question

Is $\beta < \alpha + 1$ *sharp for parametric rates?*

Partial Answer



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Theorem 2

Let $0 < \alpha < \beta$. *Then*

(i) $\mu = (\nabla\phi)_\sharp\tau$ *with* $\phi \in \Phi_{\alpha,\beta}$
$\Rightarrow \beta > \alpha + 2$

(ii) $\forall \delta > 0\ \exists \beta \leq \alpha + 2 + \delta$ *such that*
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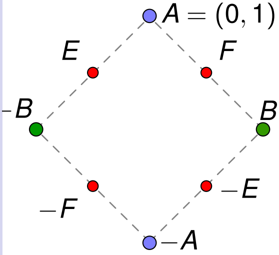

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Hence $\beta \leq \alpha + 2$ is a realistic upper bound.

Conjecture

Under Le Gouic et al. (2022) hypotheses, with C indep. of $\mathbb{P}$,
$\mathbb{E}_{\mathbb{P}^{\otimes n}}[\mathcal{W}(\mathbb{M}_n, \tau)^2] \leq \frac{1}{n}\frac{C\,\mathbb{E}_{P\sim\mathbb{P}}[\mathcal{W}(P,\tau)^2]}{(\beta-\alpha-2)^2}$ *for all* $0 < \alpha < \beta < \alpha + 2$.

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E.g. Gower (1975), H. (2010, 2012), Dryden and Mardia (2016), $2 \leq m < k$:

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- chart at $\xi \in \mathbb{S}^{m \times (k-1)-1}$ for $\mathrm{tr}(x^T\xi) > 0$: $\phi_\xi : x \mapsto \frac{x - \mathrm{tr}(x^T\xi)\xi}{\mathrm{tr}(x^T\xi)}$.

A CLT for Procrustes Means

Theorem 3

Let $Z_1, \ldots, Z_n, Z \overset{i.i.d.}{\sim} \mathbb{P} \in \mathcal{P}(\Sigma_m^k)$ *be random shapes, that a.s. assume* $\Sigma_{[\xi]}^{**}$, $\mathbb{M}(\mathbb{P}) = \{[\xi]\}$, $\hat{\mu}_n \in \mathbb{M}_n$ *m'ble selection. Then*

$$\sqrt{n}\,\mathrm{vec}\left(\phi_\xi \circ \psi_\xi(\hat{\mu}_n)\right) \xrightarrow{\mathcal{D}} \mathcal{N}\left(0,\, H^- D H^-\right)$$

with

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Remark

The $v_2, \ldots, v_N$ *span the tangent space of* $\mathbb{S}^{N-1}$ *at* $\mathrm{vec}(\xi)$.
If $\lambda_1 - \lambda_2 \to 0$ *we loose uniqueness,* H^- *explodes, i.e. the constants deteriorate.*

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  - $r \left(\log \sqrt{n}\right)^{(1+r)/r} \left(\hat{\mu}_n - \frac{\mathrm{sign}(\hat{\mu}_n)}{\left(\log \sqrt{n}\right)^{1/r}}\right) \xrightarrow{\mathcal{D}} \mathrm{sign}(Z) \cdot \log |Z|$

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- Kroshnin (2021, Theorem 4.6.1) has a logarithmic rate Wasserstein example.

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