Fréchet Means in Infinite Dimensions

Adam Quinn Jaffe

What is the "mean" of samples $Y_1, \ldots, Y_n$ in a metric space $(\mathcal{X}, d)$?

If d is the metric given by a Hilbert space norm $\|\cdot\|$ on $\mathcal{X}$, then the sample mean $\frac{1}{n}(Y_1 + \cdots + Y_n)$ is the unique solution to:

$$\begin{cases} \text{minimize} & \frac{1}{n}\sum_{i=1}^{n} \|x - Y_i\|^2 \\ \text{over} & x \in \mathcal{X} \end{cases}$$

Depends only the metric structure of the Hilbert space!

What is the “mean” of a probability measure μ on $(\mathcal{X}, d)$?

If d is the metric given by a Hilbert space norm $\|\cdot\|$ on $\mathcal{X}$, then the expectation $\int_{\mathcal{X}} d^2(x,y)\,\mathrm{d}\mu(y)$ is the unique solution to:

$$\begin{cases} \text{minimize} & \int_{\mathcal{X}} \|x-y\|^2\,\mathrm{d}\mu(y) \\ \text{over} & x \in \mathcal{X} \end{cases}$$

Depends only the metric structure of the Hilbert space!

Define the *empirical Fréchet mean* as

$$\bar{M}_n := \operatorname*{arg\,min}_{x \in \mathcal{X}} \frac{1}{n} \sum_{i=1}^{n} d^2(x, Y_i)$$

and the *population Fréchet mean* as

$$M := \operatorname*{arg\,min}_{x \in \mathcal{X}} \int_{\mathcal{X}} d^2(x, y) \, \mathrm{d}\mu(y).$$

For this talk, assume uniquely achieved.

Do we have $\bar{M}_n \to M$ in a statistically meaningful sense?

If $\mathcal{X}$ is a Hilbert space, this follows from the classical limit theorems (SLLN, CLT, concentration inequalites, rates of convergence etc.)

Definition

We say that *the strong law of large numbers (SLLN) holds in* $(\mathcal{X}, d)$ if we have $d(\bar{M}_n, M) \to 0$ almost surely when $Y_1, \ldots, Y_n$ are IID samples.

In which metric spaces does the SLLN hold?

General results require some sort of “finite-dimensionality”:

We say that $(\mathcal{X}, d)$ is a *Heine-Borel space* if the closed balls $\bar{B}_r(x) := \{y \in \mathcal{X} : d(x, y) \leq r\}$ are compact for all $x \in \mathcal{X}, r \geq 0$.

Theorem (Schötz, 2022)

If $(\mathcal{X}, d)$ is a Heine-Borel space, then the SLLN holds in $(\mathcal{X}, d)$.

But finite-dimensionality is not necessary!

Theorem (Sturm 2003)

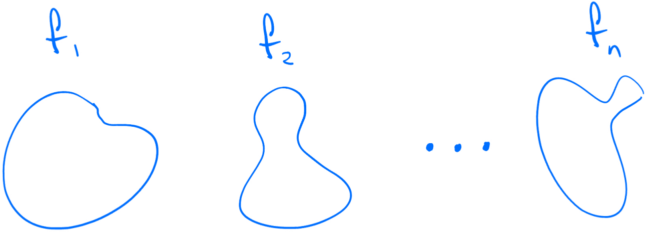
If $(\mathcal{X}, d)$ is a Hadamard space, then the SLLN holds in $(\mathcal{X}, d)$.

Theorem (Le Gouic-Loubes, 2017)

If (S, ρ) is a complete, locally compact, geodesic metric space, then the SLLN holds in the Wasserstein space $(\mathcal{P}_2(S, \rho), W_2)$.

Many other important examples of infinite-dimensional metric spaces where no asymptotic theory is known...

Example. spaces of planar loops in statistical shape analysis



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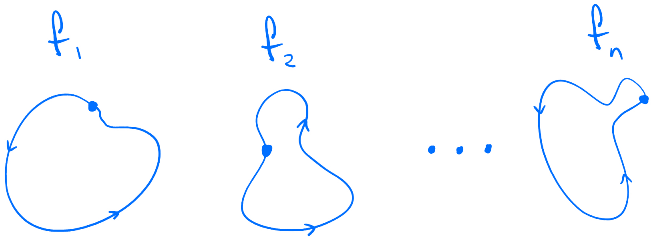

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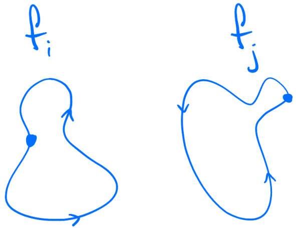

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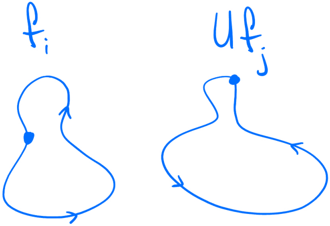

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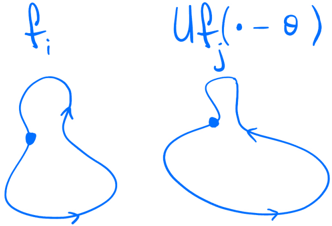

Example. spaces of planar loops in statistical shape analysis

Let $\mathcal{X}_0$ denote the space of functions $C^{1,1}$ functions $f : \mathbb{S}^1 \to \mathbb{R}^2$ satisfying $\|f'(t)\| = 1$ for all $0 \le t \le 1$.

Let d_0 denote the following pseudometric on $\mathcal{X}_0$:

$$d_0(f,g) := \min_{\substack{\theta \in \mathbb{S}^1 \\ U \in \mathrm{SO}(2)}} \left(\int_0^{2\pi} \sum_{k=0}^{2} \|U f^{(k)}(t-\theta) - g^{(k)}(t)\|^2 \, \mathrm{d}t \right)^{1/2}$$

Then, consider quotient space $(\mathcal{X}, d)$ of $(\mathcal{X}_0, d_0)$.

One of many possible metrics on spaces of planar loops used in statistical shape analysis (Kurtek-Srivastava-Klassen-Ding 2012).

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(W1) If $\{x_n\}_{n\in\mathbb{N}}$ and y in $\mathcal{X}$ satisfy $\sup_{n\in\mathbb{N}} d(x_n, y) < \infty$, then there exists a subsequence $\{n_k\}_{k\in\mathbb{N}}$ and a point $x \in \mathcal{X}$ satisfying $x_{n_k} \to x$ in w.

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We say that $(\mathcal{X}, d)$ *admits a weak convergence* if there exists a weak convergence w for $(\mathcal{X}, d)$.

Theorem (AQJ 2024)

If $(\mathcal{X}, d)$ admits a weak convergence, then the SLLN holds in $(\mathcal{X}, d)$.

Notice that the conclusion refers only to the metric d.

The existence of a weak convergence is a *geometric* property of $(\mathcal{X}, d)$.

I. Introduction

II. On Weak Convergence

III. The Continuity Theorem

IV. Future Work

II. On Weak Convergence

Basic examples:

Recall topology w on $\mathcal{X}$ is called a *weak convergence for* $(\mathcal{X}, d)$ if:

(W1) d-bounded sets are relatively w-compact,

(W2) d is w-lower-semicontinuous, and

(W3) d is w-continuous only where it is d-continuous.

metric space	weak convergence	(W1)	(W2)	(W3)
Heine-Borel space	metric convergence	definition	trivial	trivial
Hadamard space	Jost's convergence	Jost's Banach-Alaoglu theorem	weak lower semi-continuity of metric	Kadec-Klee property
Wasserstein space	weak convergence of probability measures	Prokhorov theorem	Fatou lemma	definition
uniformly convex Banach space	weak topology	Milman-Pettis theorem	weak lower semi-continuity of norm	Kadec-Klee property

Example.

Let $\mathbb{H}$ be a (possibly infinite-dimensional) Hilbert space

Let $\mathbb{K}$ denote the space of covariance operators on $\mathbb{H}$

Set $\Pi(\Sigma, \Sigma') := W_2(\mathcal{N}(0, \Sigma), \mathcal{N}(0, \Sigma'))$, the Bures-Wasserstein metric

For $\{\Sigma_n\}_{n\in\mathbb{N}}$ and Σ in $\mathbb{K}$, say $\Sigma_n \to \Sigma$ in w if

$$\int_{\mathbb{H}} \phi \, \mathrm{d}\mathcal{N}(0, \Sigma_n) \to \int_{\mathbb{H}} \phi \, \mathrm{d}\mathcal{N}(0, \Sigma)$$

for all weakly continuous $\phi : \mathbb{H} \to \mathbb{R}$.

Similar to existing considerations in the theory of gradient flows (Ambrosio-Gigli-Savaré 2008), and recovers known results for Bures-Wasserstein barycenters (Masarotto-Panaretos-Zemel 2019).

Closure properties:

Want to provide a "calculus" for constructing further examples of interest, as in Grenander's pattern theory (Mumford 2003).

metric space operation	inputs	output	weak convergence
restriction	$(\mathcal{X}, d)$ with weak convergence w, w-closed subset $\mathcal{X}' \subseteq \mathcal{X}$	$(\mathcal{X}', d)$	w
product	$(\mathcal{X}_1, d_1)$ with weak convergence w_1, $(\mathcal{X}_2, d_2)$ with weak convergence w_2	$(\mathcal{X}_1 \times \mathcal{X}_2, d_1 \otimes_q d_2)$	$w_1 \otimes w_2$
quotient	$(\mathcal{X}, d)$ with weak convergence w, compact group G acting isometrically	$(\mathcal{X}/G, d_{\mathcal{X}/G})$	Γ-convergence of orbits under w
regularization	$(\mathcal{X}, d)$ with weak convergence w, proper metric group (G, ρ) acting isometrically	$(\mathcal{X}, d_{G,\rho})$	w

Example.

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Then, consider quotient space $(\mathcal{X}, d)$ of $(\mathcal{X}_0, d_0)$.

One of many possible metrics on spaces of planar loops used in statistical shape analysis (Kurtek-Srivastava-Klassen-Ding, 2012).

III. The Continuity Theorem

Want a general asymptotic theory for Fréchet means which...

- ☑ holds in many infinite-dimensional metric spaces of interest
- ☐ implies many limit theorems of interest
- ☐ requires the minimal moment assumptions
- ☐ requires no uniqueness assumptions

Many limit theorems at once?

Notice that the empirical Fréchet mean depends only on the empirical measure $\bar{\mu}_n := \frac{1}{n}\sum_{i=1}^n \delta_{Y_i}$:

$$M = \operatorname*{arg\,min}_{x\in\mathcal{X}} \frac{1}{n}\sum_{i=1}^{n} d^2(x, Y_i)$$

So, define

$$M(\mu) := \operatorname*{arg\,min}_{x\in\mathcal{X}} \int_{\mathcal{X}} d^2(x, y)\,\mathrm{d}\mu(y).$$

Since we have $\mu_n \to \mu$ in many senses, we can deduce limit theorems for Fréchet mean sets from limit theorem from empirical measures.

Minimal moment assumption?

Write $\mathcal{P}_p(\mathcal{X})$ for the set of μ with $\int_{\mathcal{X}} d^p(x,y)\,\mathrm{d}\mu(y) < \infty$ for all $x \in \mathcal{X}$.

Define the map $M : \mathcal{P}_2(\mathcal{X}) \to 2^{\mathcal{X}}$ via

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Define the map $M : \mathcal{P}_1(\mathcal{X}) \to 2^{\mathcal{X}}$ via

$$M(\mu) := \arg\min_{x\in\mathcal{X}} \int_{\mathcal{X}} (d^2(x,y) - d^2(o,y))\,\mathrm{d}\mu(y)$$

for arbitrary $o \in \mathcal{X}$.

This makes sense because

$$|d^2(x,y) - d^2(o,y)| \leq d(x,o)(d(x,y) + d(o,y))$$

in any metric space!

Convergence without uniqueness?

For non-empty bounded subsets $\{M_n\}_{n\in\mathbb{N}}$ and M of $\mathcal{X}$, consider

$$\max_{x_n\in M_n}\min_{x\in M} d(x_n, x) \to 0.$$

Plainly, every element of M_n is close to some element of M.

If $\{M_n\}_{n\in\mathbb{N}}$ and M are singletons, then equivalent to $d(M_n, M) \to 0$.

Let W_1 denote the 1-Wasserstein metric (i.e., Kantorovich-Rubinstein metric) on $\mathcal{P}_1(\mathcal{X})$.

Theorem (AQJ 2024)

If $(\mathcal{X}, d)$ is separable and admits a weak convergence and $\{\mu_n\}_{n\in\mathbb{N}}$ and μ in $\mathcal{P}_1(\mathcal{X})$ satisfy $W_1(\mu_n, \mu) \to 0$, then

$$\max_{x_n \in M(\mu_n)} \min_{x \in M(\mu)} d(x_n, x) \to 0$$

as $n \to \infty$.

This is a purely analytic result, but we will later take $\mu_n := \bar{\mu}_n$.

Proof Outline.

Take $x_n \in M(\mu_n)$ for all $n \in \mathbb{N}$, then:

(S0) Show that $\{x_n\}_{n\in\mathbb{N}}$ is d-bounded.

(S1) Get $\{n_k\}_{k\in\mathbb{N}}$ and $x_\infty \in \mathcal{X}$ with $x_{n_k} \to x_\infty$ in w.

(S2) Show $x_\infty \in M(\mu)$.

(S3) Show $x_{n_k} \to x_\infty$ in d.

Definition

A topology w on $\mathcal{X}$ is called a *weak convergence for* $(\mathcal{X}, d)$ if:

(W1) d-bounded sets are relatively w-compact

(W2) d is w-lower-semicontinuous.

(W3) d is w-continuous only where it is d-continuous.

Earlier works (Thorpe-Theil-Johansen-Cade 2015, Le Gouic-Loubes 2017, Schötz 2022) outline same method of proof.

IV. Future Work

Verify existence of weak convergence for other metric spaces:

- large deformation diffeomorphic metric mapping (LDDMM) (Bauer-Bruveris-Michor 2014, Younes 2019)
- invariant L^2 metric on graphons (Kolaczyk-Lin-Rosenberg-Walters-Xu 2020)

Non-examples:

- Easy case $\mathcal{X} = [-1, 0) \cup (0, 1]$, with $\mu = \frac{1}{2}\delta_{-1} + \frac{1}{2}\delta_1$
- What if $\mathcal{X}$ is complete?

Refining other limit theorems:

- Central limit theorem requries some further differentiable structure
- Large deviations theory requires some additional steps

Thank you!

References

L. Ambrosio, N. Gigli, and G. Savaré. *Gradient Flows in Metric Spaces and in the Space of Probability Measures.* Lectures in Mathematics (ETH Zürich Birkhäuser), 2nd ed., 2008.

M. Bauer, M. Bruveris, and P. Michor. Overview of the geometries of shape spaces and diffeomorphism groups. *J. Math. Imag. Vis.,* 50:60-97, 2014

T. Le Gouic and J.-M. Loubes. Existence and consistency of Wasserstein barycenters. *Probab. Theory Related Fields,* 168:901-917, 2017.

E. D. Kolaczyk, L. Lin, S. Rosenberg, J. Walters, and J. Xu. Averages of unlabeled networks: geomeric characterization and asymptotic behavior. *Ann. Statist.,* 48:514-538, 2020.

S. Kurtek, A. Srivastava, E. Klassen, and Z. Ding, Statistical modeling of curves using shapes and related features. *J. Amer. Statist. Assoc.*, 107:1152-1165, 2012.

V. Masarotto, V. M. Panaretos, and Y. Zemel. Procrustes metrics on covariance operators and optimal transportation of Gaussian processes. *Sankhya A*, 8:172-213, 2019.

M. Miller and L. Younes. Group actions, homeomorphisms, and matching: a general framework. *Internat. J. Comp. Vis.,* 41:61-84, 2001.

D. Mumford. *Pattern theory: a unifying perspective.* Fields Medallists' lectures (World Scientific Publishing River Edge New Jersey), 2003.

C. Schötz. Strong laws of large numbers for generalizations of Fréchet mean sets. *Statistics,* 56(1):34-52, 2022.

K.-T. Sturm. Probability Measures on Metric Spaces of Nonpositive Curvature. *Comtemp. Math.,* 338:357-390, 2003.

M. Thorpe, F. Theil, A. M. Johansen, and N. Cade. Convergence of the k-means minimization problem using Γ-convergence. *SIAM J. Appl. Math.*, 75:2444-2474, 2015.

L. Younes. *Shapes and Diffeomorphisms.* Applied Mathematical Sciences (Springer Berlin), 2nd ed., 2019.