Finite Sample Smeariness on Spheres

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Abstract. Finite Sample Smeariness (FSS) has been recently discovered. It means that the distribution of sample Fréchet means of underlying rather unsuspicious random variables can behave as if it were smeary for quite large regimes of finite sample sizes. In effect classical quantile-based statistical testing procedures do not preserve nominal size, they reject too often under the null hypothesis. Suitably designed bootstrap tests, however, amend for FSS. On the circle it has been known that arbitrarily sized FSS is possible, and that all distributions with a non-vanishing density feature FSS. These results are extended to spheres of arbitrary dimension. In particular all rotationally symmetric distributions, not necessarily supported on the entire sphere feature FSS of Type I. While on the circle there is also FSS of Type II it is conjectured that this is not possible on higher-dimensional spheres.

1 Introduction

In non-Euclidean statistics, the Fréchet mean [Fréchet 1948] takes the role of the expected value of a random vector in Euclidean statistics. Thus an enormous body of literature has been devoted to the study of Fréchet means and its exploitation for descriptive and inferential statistics [Hendriks and Landsman 1998, Bhattacharya and Patrangenaru 2005, Huckemann 2011a, Le and Barden 2014, Bhattacharya and Lin 2017]. For the latter, it was only recently discovered that the asymptotics of Fréchet means may differ substantially from that of its Euclidean kin [Hotz and Huckemann 2015, Eltzner and Huckemann 2019]. Initially, such examples were rather exotic. Corresponding distributions have been called smeary. More recently, however, it has been discovered that also for a large class of classical distributions (e.g. all with nonvanishing densities on the circle, like, e.g. all von-Mises-Fisher distributions) Fréchet means behave in a regime up to a considerable sample sizes as if they were smeary. We call this effect finite sample smeariness (FSS), also the term lethargic means has been suggested. Among others, this effect is highly relevant for asymptotic one- and two-sample tests for equality of means. In this contribution, after making the new terminology precise, we illustrate the effect of FSS on statistical tests concerning the change of wind directions in the larger picture of climate change.

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Furthermore, while we have shown earlier that FSS of any size can be present on the circle and the torus, here we show that FSS of arbitrary size is also present on spheres of arbitrary dimension, at least for local Fréchet means. For such, on high dimensional spheres, distributions supported by barely more than a geodesic half ball may feature arbitrary high FSS. Moreover, we show that a large class of distributions on spheres of arbitrary dimension, namely all rotationally symmetric ones, e.g. all Fisher distributions, feature FSS. This means not only that the finite sample rate may be wrong, also the rescaled asymptotic variance of Fréchet means may be considerably different from the sample variance in tangent space.

2 Finite Sample Smeariness on Spheres

Let \( S^m \) be the unit sphere in \( \mathbb{R}^{m+1} \) for \( m > 1 \) and \( S^1 = [-\pi, \pi) / \sim \) with \(-\pi\) and \(\pi\) identified be the unit circle, with the distance
\[
d(x, y) = \begin{cases} 
\arccos(x^T y) & \text{for } x, y \in S^m, \\
\min\{|y - x|, 2\pi - |y - x|\} & \text{for } x, y \in S^1.
\end{cases}
\]

For random variables \( X_1, \ldots, X_n \overset{i.i.d.}{\sim} X \) on \( S^m \), \( m \geq 1 \), with silently underlying probability space \((\Omega, \mathbb{P})\) we have the Fréchet functions
\[
F(p) = \mathbb{E}[d(X, p)^2] \quad \text{and} \quad F_n(p) = \frac{1}{n} \sum_{j=1}^{n} d(X_j, p)^2 \quad \text{for } p \in S^m.
\]

We work under the following assumptions. In particular, the third Assumption below is justified by (Tran et al., 2021, Lemma 1).

**Assumptions 1** Assume that
1. \( X \) is not a.s. a single point,
2. there is a unique minimizer \( \mu = \arg\min_{p \in S^m} F(p) \), called the Fréchet population mean,
3. for \( m > 1 \), \( \mu \) is the north pole \((1, 0, \ldots, 0)\) and \( \mu = 0 \) on \( S^1 \),
4. \( \bar{\mu}_n \in \arg\min_{p \in S^m} F_n(p) \) is a selection from the set of minimizers uniform with respect to the Riemannian volume, called a Fréchet sample mean,

Note that \( \mathbb{P}\{X = -\mu\} = 0 \) for \( m > 1 \) and \( \mathbb{P}\{X = -\pi\} = 0 \) on \( S^1 \) due to (Le and Barden, 2014; Hotz and Huckemann, 2015).

**Definition 2** We have the population variance
\[
V := F(\mu) = f(0) = \mathbb{E}[d(X, \mu)^2],
\]
which, on \( S^1 \) is just the classical variance \( \mathbb{V}[X] \), and the Fréchet sample mean variance
\[
V_n := \mathbb{E}[d(\bar{\mu}_n, \mu)^2]
\]
giving rise to the modulation
\[
m_n := \frac{nV_n}{V}.
\]
We have the following finding from Hundrieser et al. (2020).

**Theorem 3** Consider $X_1, \ldots, X_n \overset{i.i.d.}{\sim} X$ on $S^1$ and suppose that $J \subseteq S^1$ is the support of $X$. Assume Assumption 4 and let $n > 1$.

Then $m_n = 1$ under any of the two following conditions

(i) $J$ is strictly contained in a closed half circle,
(ii) $J$ is a closed half circle and one of its end points is assumed by $X$ with zero probability.

Further, $m_n > 1$ under any of the two following conditions

(iii) the interior of $J$ contains a closed half circle,
(iv) $J$ contains two antipodal points, each of which is assumed by $X$ with positive probability.

Finally, suppose that $X$ has near $-\pi$ a continuous density $f$.

(v) If $f(-\pi) = 0$ then $\lim_{n \rightarrow \infty} m_n = 1$,
(vi) if $0 < f(-\pi) < \frac{1}{2\pi}$ then $\lim_{n \rightarrow \infty} m_n = \frac{1}{(1-f(-\pi)2\pi)^2} > 1$.

In Hotz and Huckemann (2015) it has been shown that $f(-\pi)2\pi$ can be arbitrary close to 1, i.e. that $\lim_{n \rightarrow \infty} m_n$ can be arbitrary large. In fact, whenever $f(-\pi)2\pi = 1$, then $\lim_{n \rightarrow \infty} m_n = \infty$. These findings give rise to the following.

**Definition 4** We say that $X$ is

(i) Euclidean if $m_n = 1$ for all $n \in \mathbb{N}$,
(ii) finite sample smeary if $1 < \sup_{n \in \mathbb{N}} m_n < \infty$,
    (i$\alpha_1$) Type I finite sample smeary if $\lim_{n \rightarrow \infty} m_n > 1$,
    (i$\alpha_2$) Type II finite sample smeary if $\lim_{n \rightarrow \infty} m_n = 1$,
(iii) smeary if $\sup_{n \in \mathbb{N}} m_n = \infty$.

3 Why is Finite Sample Smeariness called Finite Sample Smeariness?

Under FSS on the circle in simulations we see typical shapes of modulation curves in Figure 1. For statistical testing, usually building on smaller sample sizes, as detailed further in Section 4 the initial regime is decisive, cf. Figure 2.

There are constants $C_+, C_-, K > 0$, $0 < \alpha_- < \alpha_+ < 1$ and integers $1 < n_- < n_+ < n_0$ satisfying $C_+ n_+^{\alpha_+} \leq C_- n_-^{\alpha_-}$, such that

(a) $\forall n \in [n_-, n_+] \cap \mathbb{N} : 1 < C_- n_-^{\alpha_-} \leq m_n \leq C_+ n_+^{\alpha_+}$.
(b) $\forall n \in [n_0, \infty) \cap \mathbb{N} : m_n \leq K$. 

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Fig. 1: Modulation $m_n$ for von Mises distribution (Mardia & Jupp, 2000) with mean $\mu = 0$ and concentration $\kappa = 1/2$ (left), conditioned on $[-\pi + 0.2, \pi - 0.2]$ (center), and conditioned on $[-\pi, \pi + 0.1] \cup [-\pi + 0.2, \pi + 0.2] \cup [\pi - 0.1, \pi]$ (right). The dashed lines represent the respective limits of $m_n$ obtained by Theorem 3 (v), (vi).

Although under FSS, $m_n$ is eventually constant, i.e. the asymptotic rate of $\hat{\mu}_n$ is the classical $n^{-1/2}$, for nonvanishing intervals of sample sizes $[n_-, n_+]$, the “finite sample” rate is (in expectation) between

$$\left(n^{-\frac{1}{2}} < \right) n^{-\frac{1}{2} - \frac{1}{2} - \alpha} \quad \text{and} \quad n^{-\frac{1}{2} - \frac{1}{2} + \alpha},$$

i.e. like a smeary rate, cf. [Hundrieser et al. (2020)].

Of course, as illustrated in Figure 1, the modulation curve can be subject to different regimes of $\alpha-$ and $\alpha+$, in applications, typically the first regime is of interest, cf. Section 4.

Fig. 2: Schematically illustrating the modulation curve $n \mapsto m_n$ for FSS on the circle. Along $[n_-, n_+]$ the curve is between the lower ($C_- n_+^{\alpha-}$) and upper ($C_+ n_+^{\alpha+}$) bounds (dashed), satisfying the condition $C_+ n_+^{\alpha+} \leq C_- n_+^{\alpha-}$, and for $n \geq n_0$ it is below the horizontal upper bound (dashed).
4 Correcting for Finite Sample Smeariness in Statistical Testing

The central limit theorem by Hendriks and Landsman (1998) and Bhattacharya and Patrangenaru (2005) for an $m$-dimensional manifold $M$, cf. also Huckemann (2011a,b); Bhattacharya and Lin (2017) for sample Fréchet means $\hat{\mu}_n$, has been extended by Eltzner and Huckemann (2019) to random variables no longer avoiding arbitrary neighborhoods of possible cut points of the Fréchet mean $\mu$. Under nonsmeariness it has the following form:

$$\sqrt{n} \phi(\hat{\mu}_n) \stackrel{D}{\rightarrow} N(0, 4H^{-1}\Sigma H^{-1}) .$$

Here $\phi$ is a local chart mapping $\mu$ to the origin, $H$ is the expected value of the Hessian of the Fréchet function $F$ from (1) in that chart at $\mu$ and $\Sigma$ is the covariance of $\phi(X)$. In practical applications, $H$ is usually ignored, as it has got no straightforward plugin estimators, and $4H^{-1}\Sigma H^{-1}$ is simply estimated by the empirical covariance $\hat{\Sigma}_n$ of $\phi(X_1), \ldots, \phi(X_n)$ giving rise to the approximation

$$n\phi(\hat{\mu}_n)^T \hat{\Sigma}_n^{-1} \phi(\hat{\mu}_n) \stackrel{D}{\rightarrow} \chi^2_m,$$  

(2)  

E.g. Bhattacharya and Patrangenaru (2005); Bhattacharya and Lin (2017). For finite samples sizes, this approximation depends crucially on

$$m_n = \frac{\mathbb{E}[n\|\phi(\hat{\mu}_n)\|^2]}{\mathbb{E}[\text{trace}(\hat{\Sigma}_n)]} = 1 ,$$

and it is bad in regimes whenever $m_n \gg 1$. This is illustrated in Figure 3 where two samples from von Mises distributions with concentration $\kappa = 1/2$ are tested for equality of Fréchet means. Indeed the quantile based test does not keep the nominal level, whereas the bootstrap based test, see Eltzner and Huckemann.
Table 1: Comparing $p$-values of the quantile based test for equality of means of yearly wind data from Basel (Figure 4), based on \( (2) \) with the bootstrap test amending for FSS proposed in [Hundrieser et al. (2020)] for \( B = 10.000 \) bootstrap realizations.

| Test Type          | 2018 vs. 2019 | 2019 vs. 2020 | 2018 vs. 2020 |
|--------------------|---------------|---------------|---------------|
| Quantile based test| 0.00071       | 0.27          | 0.019         |
| Bootstrap based test| 0.047       | 0.59          | 0.21          |

Moreover, Table 1 shows a comparison of $p$-values of the quantile test based on \( (2) \) and the suitably designed bootstrap test for daily wind directions taken at Basel for the years 2018, 2019, and 2020, cf. Figure 4. While the quantile based test asserts that the year 2018 is highly significantly different from 2019 and 2020, the bootstrap based test shows that a significant difference can be asserted at most for the comparison between 2018 and 2019. The reason for the difference in $p$-values between quantile and bootstrap based test is the presence of FSS in the data, i.e. \( m_n \gg 1 \). Indeed, estimating for \( n = 365 \) the modulation \( m_n \) of the yearly data using \( B = 10.000 \) bootstrap repetitions, as further detailed in [Hundrieser et al. (2020)], yields \( m_{2018} = 2.99 \), \( m_{2019} = 2.97 \), and \( m_{2020} = 4.08 \).

5 Finite Sample Smeariness Universality

Consider \( p \in S^m \) parametrized as \((\theta, \sin \theta q) \in S^m \) where \( \theta \in [0, \pi] \) denotes distance from the north pole \( \mu \in S^m \) and \( q \in S^{m-1} \), which is rescaled by \( \sin \theta \).

**Theorem 5** Let \( m \geq 4 \), \( Y \) uniformly distributed on \( S^{m-1} \) and \( K > 1 \) arbitrary. Then there are \( \theta^* \in (\pi/2, \pi) \) and \( \alpha \in (0, 1) \) such that for every \( \theta \in (\theta^*, \pi) \) a random variable \( X \) on \( S^m \) with \( \Pr\{X = (\theta, \sin \theta Y)\} = \alpha \) and \( \Pr\{X = \mu\} = 1 - \alpha \) features \( \sup_{n \in \mathbb{N}} m_n \geq \lim_{n \to \infty} m_n > K \). In particular, \( \theta^* = \frac{\pi}{2} + \mathcal{O}(m^{-1}) \).
Proof. The first assertion follows from [Eltzner 2020, Theorem 4.3] and its proof in Appendix A.5 there. Notably \( \theta^* = \theta_{m,A} \) there. The second assertion has been shown in [Eltzner 2020, Lemma A.5].

**Theorem 6** Let \( X \) be a random variable on \( \mathbb{S}^m \) with \( m \geq 2 \) with unique nonsmeary mean \( \mu \), which is invariant under rotation around \( \mu \) and which is not a point mass at \( \mu \). Then \( \mu \) is Type I finite sample smeary.

Proof. From [Eltzner 2020], page 17, we see that the Fréchet function \( F_\theta \) for a uniform distribution on the \( \mathbb{S}^{m-1} \) at polar angle \( \theta \) evaluated at a point with polar angle \( \psi \) from the north pole is

\[
a(\psi, \theta, \phi) := \arccos (\cos \psi \cos \theta + \sin \psi \sin \theta \cos \phi)
\]

\[
F_\theta(\psi) = \left( \int_0^{2\pi} \sin^{m-2} \phi \, d\phi \right)^{-1} \int_0^{2\pi} \sin^{m-2} \phi \, a^2(\psi, \theta, \phi) \, d\phi.
\]

Defining a probability measure \( d\mathbb{P}(\theta) \) on \( [0, \pi] \), the Fréchet function for the corresponding rotation invariant random variable is

\[
F(\psi) = \int_0^\pi F_\theta(\psi) \, d\mathbb{P}(\theta).
\]

On page 17 of [Eltzner 2020] the function

\[
f_2(\theta, \psi) := \frac{1}{2} \sin^{m-1} \theta \int_0^{2\pi} \sin^{m-2} \phi \, d\phi \frac{d^2}{d\psi^2} F_\theta(\psi)
\]

is defined and from Equation (5) on page 19 we can calculate

\[
f_2(\theta, 0) = \sin^{m-2} \theta \left( \frac{1}{m - 1} \sin \theta + \theta \cos \theta \right) \int_0^{2\pi} \sin^m \phi \, d\phi
\]

\[
= \sin^{m-1} \theta \int_0^{2\pi} \sin^{m-2} \phi \, d\phi \left( \frac{1}{m} + \frac{m - 1}{m} \theta \cot \theta \right),
\]

which yields the Hessian of the Fréchet function for \( d\mathbb{P}(\theta) \) as

\[
\text{Hess} F(0) = 2\text{Id}_m \int_0^\pi \left( \frac{1}{m} + \frac{m - 1}{m} \theta \cot \theta \right) \, d\mathbb{P}(\theta).
\]

One sees that \( \theta \cot \theta \leq 0 \) for \( \theta \geq \pi/2 \). For \( \theta \in (0, \pi/2) \) we have

\[
\tan \theta > \theta \quad \iff \quad \theta \cot \theta < 1 \quad \iff \quad \left( \frac{1}{m} + \frac{m - 1}{m} \theta \cot \theta \right) < 1.
\]

Using \( \Sigma[\mu] \) to denote the CLT limit \( n \text{Cov}[\hat{\mu}_n] \to \Sigma[\mu] \), cf. [Bhattacharya and Patrangenaru 2005], we get the result

\[
\text{Hess} F(\mu) < 2\text{Id}_m \quad \Rightarrow \quad \Sigma[\mu] > \text{Cov} \left[ \log \mu X \right] \quad \Rightarrow \quad \text{trace} (\Sigma[\mu]) > \text{Var}[X].
\]

The claim follows at once.
Conjecture 7 Let $X$ be a random variable supported on a set $A \subset \mathbb{S}^m$ whose convex closure has nonzero volume and which has a unique mean $\mu$. Then $\mu$ is Type I finite sample smeary.

Bibliography

Bhattacharya, R. and L. Lin (2017). Omnibus CLTs for Fréchet means and nonparametric inference on non-Euclidean spaces. *Proceedings of the American Mathematical Society* 145(1), 413–428.

Bhattacharya, R. N. and V. Patrangenaru (2005). Large sample theory of intrinsic and extrinsic sample means on manifolds II. *The Annals of Statistics* 33(3), 1225–1259.

Eltzner, B. (2020). Geometrical smeariness – a new phenomenon of Fréchet means. arXiv:1908.04233v3.

Eltzner, B. and S. Huckemann (2017). Bootstrapping descriptors for non-euclidean data. In *Geometric Science of Information 2017 proceedings*, 12–19. Springer.

Eltzner, B. and S. F. Huckemann (2019). A smeary central limit theorem for manifolds with application to high-dimensional spheres. *The Annals of Statistics* 47(6), 3360–3381.

Fréchet, M (1948). Les éléments aléatoires de nature quelconque dans un espace distancié. *Annales de l’Institut de Henri Poincaré* 10(4), 215–310.

Hendriks, H. and Z. Landsman (1998). Mean location and sample mean location on manifolds: asymptotics, tests, confidence regions. *Journal of Multivariate Analysis* 67, 227–243.

Hotz, T. and S. Huckemann (2015). Intrinsic means on the circle: Uniqueness, locus and asymptotics. *Annals of the Institute of Statistical Mathematics* 67(1), 177–193.

Huckemann, S. (2011a). Inference on 3D Procrustes means: Tree boles growth, rank-deficient diffusion tensors and perturbation models. *Scandinavian Journal of Statistics* 38(3), 424–446.

Huckemann, S. (2011b). Intrinsic inference on the mean geodesic of planar shapes and tree discrimination by leaf growth. *The Annals of Statistics* 39(2), 1098–1124.

Hundrieser, S., B. Eltzner, and S. F. Huckemann (2020). Finite sample smeariness of Fréchet means and application to climate. arXiv:2005.02321

Le, H. and D. Barden (2014). On the measure of the cut locus of a Fréchet mean. *Bulletin of the London Mathematical Society* 46(4), 698–708.

Mardia, K.V. and P.E. Jupp (2000). *Directional Statistics*. New York: Wiley meteoblue AG (2021) history+ platform. https://www.meteoblue.com/en/weather/archive/export/basel_switzerland_2661604. Last checked on 09/02/2021

Tran, D., B. Eltzner, and S. F. Huckemann (2021). Smeariness begets finite sample smeariness. *submitted to GSI 2021*