Measure Dependent Asymptotic Rate of the Mean: Geometrical Smeariness

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Abstract

The central limit theorem (CLT) for the mean in Euclidean space features a normal limiting distribution and an asymptotic rate of $n^{-1/2}$ for all probability measures it applies to. We revisit the generalized CLT for the Fréchet mean on hyperspheres. It has been found by Eltzner and Huckemann (2019) that for some probability measures, the sample mean fluctuates around the population mean asymptotically at a scale $n^{-\alpha}$ with exponent $\alpha = 1/6$ with a non-normal distribution. This is at first glance in analogy to the situation on a circle, described by Hotz and Huckemann (2015). In this article we show that the phenomenon on hyperspheres of higher dimension is qualitatively different, as it does not rely on topological, but geometrical properties on the space, namely on the curvature, not on probability mass near the cut locus. This also leads to the conjecture that probability measures for which the asymptotic rate of the mean is $\alpha = 1/6$ are possible more generally in positively curved spaces.

1 Introduction

The central limit theorem is a cornerstone of frequentist statistics. Building on this fundamental theorem for real random variables, asymptotic theory has been developed to encompass random variables in a wide variety of data spaces including vector spaces (presented in many textbooks, e.g. Mardia et al. (1979)) and spaces like manifolds, e.g. Bhattacharya and Patrangenaru (2003, 2005); Bhattacharya and Bhattacharya (2012), and stratified spaces, e.g. Barden et al. (2013); Hotz et al. (2013). While the standard central limit theorem features a normal limiting distribution and an asymptotic rate of $n^{-1/2}$, cases with other limiting distributions and other convergence behavior have been studied.

The last two decades have especially seen the development of asymptotic theory for Fréchet means and also more general m-estimators on non-Euclidean data spaces Bhattacharya and Patrangenaru (2003, 2005); Bhattacharya and Bhattacharya (2008); Huckemann (2011b,a); Bhattacharya and Bhattacharya (2012). These developments are based on the formulation of the mean in Euclidean space and general metric spaces as an m-estimator by Fréchet.

This has lead to the discovery of phenomena like “smeariness” Hotz and Huckemann (2015), where the asymptotic rate is lower than $n^{-1/2}$. This phenomenon has been firmly rooted in asymptotic theory by the author and collaborators using empirical process theory, see Eltzner and Huckemann (2019). Another striking phenomenon concerning mean estimators on positively curved spaces was dubbed “stickiness” of mean estimators on stratified spaces Hotz et al. (2013); Barden et al. (2013, 2018), where convergence to the population mean exceeds every asymptotic rate and the population mean will exactly reach the population mean almost surely.

While lower rates of convergence than $n^{-1/2}$ are known for several estimators, these rates are usually independent of the probability measure and are a property of the estimated parameter and the data and parameter spaces. Even for heavy-tailed distributions like the Cauchy distribution in Euclidean space, the generalized CLT for $\alpha$-stable distributions features an asymptotic rate of $n^{-1/2}$, albeit with

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different limiting distributions. Smeariness, on the other hand, occurs for the simple plug-in estimator of the Fréchet mean but it is not a property of the definition of the mean. Instead, it occurs for some probability measures, but not for others and a wide range of asymptotic rates can be realized for different measures on the circle, see Hotz and Huckemann (2015); Hundrieser (2017). This sets smeariness apart from previously known cases of lower rates of estimator convergence, since knowing the space and the estimator will no longer establish an asymptotic rate to be expected.

Asymptotic theory is underpinning the theory of asymptotic statistical tests. Many widely used approximations for the quantiles of test statistics, used for example in the t-test, are derived from asymptotic considerations. In this sense, asymptotic theory is not only of mathematical interest but also has immediate practical importance. A second important application of asymptotic theory is the theoretical foundation of bootstrap methods. These have tremendously increased in importance with the advent of powerful computers for two reasons. Firstly, computers enable quick resampling and thus essentially make bootstrapping possible. Secondly, the possibility of quick numerical optimization makes the usage of more complex data types and estimators possible, which cannot always be determined in closed form. As a result, the bootstrap is often the only way to achieve estimators e.g. for the covariance of a complex estimator or for standard t-like test statistics based thereon. Therefore, understanding smeariness is of vital importance for data analysis of spaces of positive curvature.

In the present article we will show that smeariness on higher dimensional hyperspheres is not linked to any specific value of probability density at the cut locus of the mean. In fact, it can even occur, if no probability mass is present in a finite neighborhood of the cut locus. In a brief introductory section, we introduce the necessary terminology and theory and thoroughly reviewing the existing literature. We then establish the notion of geometrical smeariness in contrast to topological smeariness. We give an example of geometrical smeariness and explain its significance.

2 Fréchet Means and M-Estimators

We recall some of the very specialized tools and terminology which are necessary to state our results. Furthermore, we will very briefly recall previous results on smeariness.

2.1 Basic Notions

First, we introduce some basic notions, which will be used throughout the text. None of this is original and all the objects defined here are widely known in the field. This section only serves to fix notation. In all of the following let $Q$ be a topological space called the data space and $P$ a topological space with continuous metric function $d$ called the parameter space. $\Omega$ is a probability space as usual. Let $\rho : P \times Q \to \mathbb{R}$ a continuous function, $X : \Omega \to Q$ a $Q$-valued random variable.

**Definition 2.1.** For given $\rho$ and $X$ we define the population and sample Fréchet functions $F$ and $F_n$, the population and sample Fréchet variances $V$ and $V_n$ and the set of population and sample descriptors $E$ and $E_n$ as follows

\[
F(p) = \mathbb{E}[\rho(p,X)] \\
F_n(\omega,p) = \frac{1}{n} \sum_{i=1}^{n} \rho(p,X_i(\omega)) \hspace{1cm} (1) \\
V = \inf_{p \in P} F(p) \\
V_n(\omega) = \inf_{p \in P} F_n(\omega,p) \hspace{1cm} (2) \\
E = \{p \in P : F(p) = \ell\} \\
E_n(\omega) = \{p \in P : F_n(\omega,p) = \ell_n(\omega)\} \hspace{1cm} (3)
\]

If $E$ and $E_n$ are non-empty, the elements of $E_n$ are called m-estimators. The argument $\omega$ will be suppressed in the following unless it is important for understanding the text.

**Notation 2.2.** For a point $p \in P$ and $\varepsilon > 0$ let $B_\varepsilon(p) = \{p' \in P : d(p,p') < \varepsilon\}$.

**Definition 2.3.** Consider a point in a Riemannian manifold $p \in M$. The cut locus $\text{Cut}(p)$ of $p$ is the closure of the set of all points $q \in M$ such that there is more than one shortest geodesic from $p$ to $q$. 

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Remark 2.4. For the circle and spheres of arbitrary dimension, the cut locus of a point \( p \) is simply its antipodal point. However, for the torus \( S^1 \times S^1 \) the cut locus of a point \((p_1, p_2)\) is the union of the two circles corresponding to \( \text{Cut}(p_1) \) and \( \text{Cut}(p_2) \) and intersecting at the antipode \((\text{Cut}(p_1), \text{Cut}(p_2))\). More generally, the cut locus of a torus of dimension \( m \) always has dimension \( m - 1 \).

Since we consider asymptotics, we consider a Riemannian manifold \( \tilde{P} \) as parameter space. In order to define a CLT for random vectors, we will usually transition to a euclidean parameter space \( P \subset T_{p_0} \tilde{P} \) in the tangent space of some point \( p_0 \in \tilde{P} \) using the exponential map.

Definition 2.5. For a Riemannian manifold \( P \) and a point \( p \in P \) we define the exponential map \( \exp_p : T_pP \to P \). This is the unique map with \( \exp_p(0) = p \) and for any \( v \in T_pP \) we consider the arc length parametrized geodesic \( \gamma \) with \( \gamma(0) = p \) and \( \gamma'(0) = \frac{v}{|v|} \) and set \( \exp_p(v) = \gamma(|v|) \). The inverse of the exponential map \( \exp_p \), which exists outside of \( \text{Cut}(p) \), is called the logarithm map and is denoted by \( \log_p \). It maps the point \( q \in P \) to a vector in the tangent space \( T_pP \) whose length is the same as the geodesic distance between \( p \) and \( q \).

Definition 2.6 (Local Manifold Parameter Space). Assume that there is a neighborhood \( \tilde{U} \) of \( p_0 \in \tilde{P} \), \( m \in \mathbb{N} \), such that with a neighborhood \( P \subset T_{p_0}\tilde{P} \) of the origin in \( T_{p_0}\tilde{P} \cong \mathbb{R}^m \) the exponential map \( \exp_{p_0} : P \to \tilde{U} \), \( \exp_{p_0}(0) = p_0 \), is a diffeomorphism. We set for \( p = \exp_{p_0}(x), p' = \exp_{p_0}(x') \in \tilde{U} \) and \( q \in Q \),

\[
\rho : (x, q) \mapsto \bar{p}(\exp_{p_0}(x), q),
\]

\[
F : x \mapsto \bar{F}(\exp_{p_0}(x)),
\]

\[
F_n : x \mapsto \bar{F}_n(\exp_{p_0}(x)).
\]

In the following, we will only consider population minimizers \( p_0 \in \bar{E} \) as reference points for such local linear parameter spaces.

Remark 2.7. The construction in Definition 2.6 implies a reduction of the parameter space, since \( \exp_{p_0}(P) \subset \tilde{P} \) is usually a true subset, often of finite volume. Whenever we use this construction, we therefore need to make sure that a restriction of the parameter space to a neighborhood of a certain parameter \( p_0 \) is compatible with the argument we would like to make. We will make use of strong consistency results, i.e. laws of large numbers, to this end.

Definition 2.8. Let \( P = Q \) and \( \rho(p, X) := d_Q^2(p, X) \) where \( d_Q \) is a metric on \( Q \), then a Fréchet \((L_2)\) mean \( \mu \) for a random variable \( X \) is any element of \( E \). In all of the following, whenever \( Q \) is a Riemannian manifold, \( d_Q \) will be the geodesic distance with respect to the metric tensor of \( Q \).

2.2 Smeariness

Smeariness was first described for the Fréchet mean on the circle by Hotz and Huckemann (2015). While for other estimators a slower rate of convergence to the population mean than \( n^{1/2} \) had been well known, the appearance of such a rate for the Fréchet mean in finite dimension was surprising. We will here define the concept of smeariness in a rather general way for \( m \)-estimators following Eltzner and Huckemann (2019).

Definition 2.9. Consider an \( m \)-estimation with \( Q \) and \( P \) being manifolds with a unique population minimizer \( \mu \), such that \( E = \{ \mu \} \) and consider any measurable selection \((\hat{\mu}_n \in E_n)_n\). Then the estimator has a lower asymptotic rate, if there is a \( 0 < \tau < 1/2 \) such that

\[
n^\tau \log_n(\hat{\mu}_n) = O_p(1).
\]

However, one may consider this definition too broad for the term “smeariness” as it summarizes all cases of slower asymptotic rates, even ones that were known well before the term “smeariness” was coined. To make our definition more specific, we revisit a crucial lemma for the proof of the CLT. In the following, we will work with a manifold parameter space an we will use the exponential coordinate construction from Definition 2.6 around the unique population mean \( \mu \) to simplify the treatment. As noted above, this means that we assume an asymptotic consistency result to hold.
Lemma 2.10 (van der Vaart (2000) Theorem 5.52). Assume that for fixed constants $C$ and $\alpha > \beta$ for every $n$ and for sufficiently small $\delta$

\[
\sup_{||x|| < \delta} |F(x) - F(0)| \geq C \delta^\alpha,
\]

(4)

\[
\mathbb{E}^* \left( n^{1/2} \sup_{||x|| < \delta} \left| F_n(x) - F(x) - F_n(0) + F(0) \right| \right) \leq C \delta^\beta.
\]

(5)

Then, any a random sequence $B_\delta(0) \ni y_n \xrightarrow{P} 0$ that satisfies $F_n(y_n) \leq F_n(0)$ exhibits an asymptotic rate of convergence $n^{1/(2\alpha - 2\beta)} y_n = \mathcal{O}_P(1)$.

In any proof of an asymptotic result relying on Lemma 2.10, there are thus two possible causes for a slower rate of convergence. The first is a higher order $\alpha > 2$ of the first non-vanishing term in the power series expansion of the Fréchet function around $\mu$. The second is a lower order $\beta < 1$ of the empirical process when approaching $\mu$. Smeariness in the stricter sense is only concerned with the former case. We will therefore introduce a more restrictive definition of smeariness, which specifies properties of the Fréchet function near $\mu$.

Definition 2.11. Consider an $m$-estimation with $Q$ and $P$ being manifolds with a unique population minimizer $\mu$, such that $E = \{\mu\}$ and consider any measurable selection $(\hat{\mu}_n \in E_n)_n$. Furthermore, we require that there is a $\zeta > 0$ such that $\forall x \in \partial B_\zeta(0) : F(x) > F(0)$. Then the estimator is smeary, if with $2 \leq r \in \mathbb{R}$, a rotation matrix $R \in SO(m)$ and $T_1, \ldots, T_m > 0$ the Fréchet function admits the power series expansion

\[
F(x) = F(0) + \sum_{j=1}^m T_j |(Rx)_j|^r + o(||x||^r).
\]

(6)

In this article we will distinguish two different classes of smeary estimators with different properties. The first smeary estimator, which has been described by Hotz and Huckemann (2015), is the Fréchet mean on the circle. In this case, a critical density at the cut locus of the mean plays a crucial role.

For smeary asymptotics to occur at the Fréchet mean $\mu$ on the circle, the probability density at the antipode $\text{Cut}(\mu)$ of the mean $\mu$ must equal the uniform probability density, which is $\frac{1}{2\pi}$ on an $S^1$ parametrized in radians. The exponent $r$ in Definition 2.11 is determined by the rate with which the probability density approaches $\frac{1}{2\pi}$ from below when approaching $\text{Cut}(\mu)$, as elaborated in Hotz and Huckemann (2015); Hundrieser (2017). In the flat torus, this critical density must be realized for all marginals, see Hundrieser (2017).

The second class of smeary estimators as described by Eltzner and Huckemann (2019) are Fréchet means on hyperspheres of arbitrary dimension. While the probability measures discussed by Eltzner and Huckemann (2019) all feature a non-vanishing density at the antipode of the mean, the question whether smeariness depends on a critical density at the antipode in this case was left open. In the present article, we will show that no critical density exists and in fact smeariness can even occur, if there is no probability mass in a neighborhood of finite size around the antipode of the mean.

3 Geometrical Smeariness

While smeary probability measures were described for spheres of any dimension by Eltzner and Huckemann (2019), it is not clear, whether the probability density which these measures exhibit at the cut locus of the mean bear any significance or if they can be arbitrary. In this section, we will show that for spheres of higher dimension than one, smeary measures exist which have vanishing probability density within a neighborhood of the cut locus of the mean. This illustrates that smeariness on spheres is profoundly different from smeariness on circles or tori.
3.1 Smeariness on Hyperspheres

In this section, we will present a probability measure on hyperspheres of dimension $m \geq 5$ which exhibits smeariness despite the fact that a neighborhood of the cut locus of the mean does not contain any probability mass. To provide motivation and lay some computational ground work for this model, we will first consider the simpler model already discussed in Eltzner and Huckemann (2019). We will then replicate some of the calculations already carried out there and add some observations which we will need for our more sophisticated model.

3.1.1 A Simpler Model

Consider a random variable $X$ distributed on the $m$-dimensional unit sphere $S^m$ ($m \geq 2$) that is uniformly distributed on the lower half sphere $L^m = \{ q \in S^m : q_2 \leq 0 \}$ with total mass $0 < \alpha < 1$ and assuming the north pole $\mu = (0, 1, 0, \ldots, 0)^T$ with probability $1 - \alpha$. Then we have the Fréchet function

$$ F : S^m \to [0, \infty), \quad p \mapsto \int_{S^m} \tilde{\mu}(p, q) \, d\mathbb{P}^X(q) $$

involving the squared spherical distance $\tilde{\mu}(p, q) = \arccos(p, q)^2$ based on the standard inner product $\langle \cdot, \cdot \rangle$ of $\mathbb{R}^{m+1}$. Every minimizer $p^* \in S^m$ of $F$ is called an intrinsic Fréchet population mean of $X$.

Define the volume $V_m$ of $S^m$ and the parameter $\gamma_m$ used below

$$ V_m = \text{vol}(S^m) = \frac{2\pi^{\frac{m+1}{2}}}{\Gamma\left(\frac{m+1}{2}\right)}, \quad \gamma_m = \frac{V_{m+1}}{2V_m} = \frac{\sqrt{\pi} \Gamma\left(\frac{m+1}{2}\right)}{2 \Gamma\left(\frac{m+1}{2}\right)}.$$

Moreover, we have the exponential chart centered at $\mu \in S^m$ with inverse

$$ \exp_{\mu}^{-1}(p) = (e_1, e_3, \ldots, e_{m+1})^T \left( p - \langle p, \mu \rangle \mu \right) \frac{\arccos(p, \mu)}{\|p - \langle p, \mu \rangle \mu\|} = x \in \mathbb{R}^m $$

where $e_1, \ldots, e_{m+1}$ are the standard unit column vectors in $\mathbb{R}^{m+1}$. Note that $\exp_{\mu}^{-1}$ has continuous derivatives of any order in $\tilde{U} = S^m \setminus \{ -\mu \}$ and recall that $e_2 = \mu$.

In this model with $\mu = e_2$, we can simplify calculations considerably by choosing polar coordinates $\theta_1, \ldots, \theta_{m-1} \in [-\pi/2, \pi/2]$ and $\phi \in [-\pi, \pi]$ in the non-standard way

$$ q = \begin{pmatrix} q_1 \\ q_2 \\ \vdots \\ q_{m-1} \\ q_m \\ q_{m+1} \end{pmatrix} = \begin{pmatrix} -\left( \prod_{j=1}^{m-1} \cos \theta_j \right) \cos \phi \\ -\left( \prod_{j=1}^{m-1} \cos \theta_j \right) \sin \phi \\ \vdots \\ -\cos \theta_1 \cos \theta_2 \sin \theta_3 \\ -\cos \theta_1 \sin \theta_2 \\ \sin \theta_1 \end{pmatrix}, $$

such that the north pole $\mu$ has coordinates $(0, \ldots, 0, -\pi/2)$. In these coordinates, we may assume w.l.o.g. that the arbitrary but fixed point $p \in S^m$ has coordinates $(0, 0, \ldots, 0, -\pi/2 + \psi)$ with suitable $\psi \in [0, \pi]$. Setting $\Theta = [-\pi/2, \pi/2]$, defining the functions

$$ u : \Theta^{m-1} \to [0, 1], \quad \theta = (\theta_1, \ldots, \theta_{m-1}) \mapsto \prod_{j=1}^{m-1} \cos^{m-j} \theta_j \quad v(\theta) = \prod_{j=1}^{m-1} \cos \theta_j, $$

we have the spherical volume element $g(\theta) \, d\theta \, d\phi$. Furthermore, we have that

$$ \tilde{F}(p) = \psi^2 (1 - \alpha) + \tilde{F}(\mu) + \frac{2\alpha}{V_m} \left( C_+ (\psi) - C_- (\psi) \right) =: F(\psi) $$

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with the two “crescent” integrals
\[
C_+ (\psi) = \int_{\Omega_{m-1}} u(\theta) \int_{- \psi}^0 \hat{\rho}(\theta, q)^2 d\phi d\theta = \int_{\Omega_{m-1}} u(\theta) \int_{- \psi}^\psi \left( \arccos \left( v(\theta) \sin \phi \right) \right)^2 d\phi d\theta
\]
\[
C_- (\psi) = \int_{\Omega_{m-1}} u(\theta) \int_{\pi - \psi}^\pi \hat{\rho}(\theta, q)^2 d\phi d\theta = \int_{\Omega_{m-1}} u(\theta) \int_{- \psi}^\psi \left( \arccos \left( -v(\theta) \sin \phi \right) \right)^2 d\phi d\theta
\]

because the spherical measure of \(L^m\) is \(V_m/2\).

Since for \(a \in [0, 1]\),
\[
(\arccos(a))^2 - (\arccos(-a))^2 = (\arccos(a) + \arccos(-a))(\arccos(a) - \arccos(-a)) = 2\pi \left( \frac{\pi}{2} - \arccos(a) \right) = -2\pi \arcsin(a),
\]

which has arbitrary derivatives if \(-1 < a < 1\), we have that
\[
\tilde{F} \circ \exp_\mu(x) = F(\psi) = \psi^2(1 - \alpha) + F(0) - \frac{4\pi \alpha}{V_m} \int_{\Omega_{m-1}} u(\theta) \int_0^\psi \arcsin(\psi(\theta) \sin \phi) d\phi d\theta \tag{7}
\]

for every \(x \in \exp^{-1}(\tilde{U})\) with \(||x|| = \psi\).

Consider the derivatives
\[
F'(\psi) = 2\psi(1 - \alpha) - \frac{4\pi \alpha}{V_m} \int_{\Omega_{m-1}} u(\theta) \arcsin \left( v(\theta) \sin \psi \right) d\theta,
\]
\[
F''(\psi) = 2(1 - \alpha) - \frac{4\pi \alpha}{V_m} \int_{\Omega_{m-1}} u(\theta) v(\theta) \frac{\cos \psi}{\sqrt{1 - v(\theta)^2 \sin^2 \psi}} d\theta,
\]
\[
F^{(3)}(\psi) = \frac{4\pi \alpha}{V_m} \int_{\Omega_{m-1}} u(\theta) v(\theta) \frac{(1 - v(\theta)^2) \sin \psi}{(1 - v(\theta)^2 \sin^2 \psi)^{3/2}} d\theta,
\]
\[
F^{(4)}(\psi) = \frac{4\pi \alpha}{V_m} \int_{\Omega_{m-1}} u(\theta) v(\theta) (1 - v(\theta)^2) \frac{(1 + 2v(\theta)^2 \sin^2 \psi) \cos \psi}{(1 - v(\theta)^2 \sin^2 \psi)^{5/2}} d\theta.
\]

We can conclude that
\[
\forall \psi \in [0, \pi] \quad F''(\psi) \geq 2(1 - \alpha) - \frac{4\pi \alpha}{V_m} \int_{\Omega_{m-1}} u(\theta) v(\theta) d\theta = 2 - \alpha \left( 2 + \frac{V_{m+1}}{V_m} \right) = 0 \tag{8}
\]
\[
\forall \psi \in (0, \pi) \quad F^{(3)}(\psi) \geq \sin \psi \frac{4\pi \alpha}{V_m} \int_{\Omega_{m-1}} u(\theta) v(\theta) (1 - v(\theta)^2) d\theta > 0 \tag{9}
\]
\[
\forall \psi \in [0, \pi/2] \quad F^{(4)}(\psi) \geq \cos \psi \frac{4\pi \alpha}{V_m} \int_{\Omega_{m-1}} u(\theta) v(\theta) (1 - v(\theta)^2) d\theta = F^{(4)}(0) \cos \psi > 0 \tag{10}
\]
\[
\forall \psi \in [0, \pi/3] \quad F^{(4)}(\psi) \geq F^{(4)}(0) \cos \psi \geq \frac{1}{2} F^{(4)}(0). \tag{11}
\]

We recall \(F^{(4)}(0) = \frac{\alpha V_{m+1}}{V_m} \frac{m-1}{m+1} = c_m > 0\) and that the inequality in (8) is strict for \(\psi \neq 0, \pi\), due to \(0 < h(\theta) < 1\) for all \(\theta \in (-\pi/2, \pi/2)^{m-1}\). Hence we infer that \(F'(\psi)\) is strictly increasing in \(\psi\) from \(F'(0) = 0\), yielding that there is no stationary point for \(F\) other than \(p = \mu\).
3.1.2 A More General Model

For the generalized model we consider here, we cannot make use of the crescent integrals. Therefore, the
necessary calculations are somewhat more tedious. We fix the north pole \( \mu = e_{m+1} \) and use standard
coordinates

\[
q = \begin{pmatrix}
q_1 \\
q_2 \\
\vdots \\
q_{m-1} \\
q_m \\
q_{m+1}
\end{pmatrix},
\]

\[
p = \begin{pmatrix}
p_1 \\
\vdots \\
p_{m-1} \\
p_m \\
p_{m+1}
\end{pmatrix} = \begin{pmatrix}
0 \\
\vdots \\
0 \\
\sin \psi \\
\cos \psi
\end{pmatrix},
\]

where \( \mu = (0, \ldots, 0) \) in these coordinates.

Consider a random variable \( X \) distributed on the \( m \)-dimensional unit sphere \( S^m \) \((m \geq 4)\) that is
uniformly distributed on \( L^m = \{ q \in S^m : \theta \in [\pi/2, \pi - \beta] \} \) with total mass \( 0 < \alpha < 1 \) and assuming \( \mu \)
with probability \( 1 - \alpha \). Then we have the Fréchet function

\[
\tilde{F} : S^m \to [0, \infty), \quad p \mapsto \int_{S^m} \tilde{\rho}(p, q) \, dP_X(q)
\]

involving the squared spherical distance \( \tilde{\rho}(p, q) = \arccos\langle p, q \rangle \) based on the standard inner product \( \langle \cdot, \cdot \rangle \)
of \( \mathbb{R}^{m+1} \). We can write the Fréchet function as a function of \( \psi, \alpha \) and \( \beta \). To keep the calculations
readable, we introduce some shorthand notation

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

\[
h'(\psi, \theta, \phi) := \frac{\partial}{\partial \psi} h(\psi, \theta, \phi) = -\sin \psi \cos \theta + \cos \psi \sin \theta \cos \phi
\]

\[
a(\psi, \theta, \phi) := \arccos h(\psi, \theta, \phi)
\]

\[
s(\theta, \phi) := \sin \theta \sin \phi,
\]

where we will suppress the arguments in the following, and we note

\[
h''(\psi, \theta, \phi) := \frac{\partial^2 h}{\partial \psi^2} = -h \quad \text{and} \quad 1 - h^2 = (h')^2 + s^2.
\]

Now the Fréchet function can be written as

\[
F(\alpha, \beta, \psi) := (1 - \alpha)\psi^2 + \alpha g(\beta) \int_{\pi/2}^{\pi-\beta} \sin \theta \int_0^\pi s^{m-2} a^2 d\phi d\theta
\]

\[
= \psi^2 + \alpha g(\beta) \int_{\pi/2}^{\pi-\beta} \sin \theta \int_0^\pi s^{m-2} (a^2 - \psi^2) d\phi d\theta
\]

\[
g(\beta) := \left( \int_{\pi/2}^{\pi-\beta} \sin \theta \int_0^\pi s^{m-2} d\phi d\theta \right)^{-1}.
\]
By straightforward calculation we determine the first 4 derivatives with respect to $\psi$
\[
\frac{\partial F}{\partial \psi} = 2\psi - 2\alpha g(\beta) \int_{\pi/2}^{\pi-\beta} \sin \theta \int_0^\pi s^{m-2} \left( \frac{h' a}{1 - h^2} \right)^{1/2} + \psi \right) \, d\phi \, d\theta
\]
\[
\frac{\partial^2 F}{\partial \psi^2} = 2 + 2\alpha g(\beta) \int_{\pi/2}^{\pi-\beta} \sin \theta \int_0^\pi s^{m-2} \left( \frac{(h')^2}{1 - h^2} + \frac{h s^2 a}{(1 - h^2)^{3/2}} - 1 \right) \, d\phi \, d\theta
\]
\[
\frac{\partial^3 F}{\partial \psi^3} = 2\alpha g(\beta) \int_{\pi/2}^{\pi-\beta} \sin \theta \int_0^\pi s^{m} \left( \frac{-3h h'}{(1 - h^2)^2} + \frac{(1 + 2h^2) h' a}{(1 - h^2)^{5/2}} \right) \, d\phi \, d\theta
\]
\[
\frac{\partial^4 F}{\partial \psi^4} = 2\alpha g(\beta) \int_{\pi/2}^{\pi-\beta} \sin \theta \int_0^\pi s^{m} \left( \frac{3s^2 h^2 - 4(1 + 2h^2)(h')^2}{(1 - h^2)^3} + \frac{(4(2 + h^2)(h')^2 - s^2(1 + 2h^2)h a}{(1 - h^2)^{7/2}} \right) \, d\phi \, d\theta.
\]
For later use we introduce further shorthand notation (using $1 - h^2 = (h')^2 + s^2$)
\[
f_2(\theta, \psi) := \sin \theta \int_0^\pi s^{m} \left( \frac{-1}{1 - h^2} + \frac{h a}{(1 - h^2)^{3/2}} \right) \, d\phi
\]
\[
f_3(\theta, \psi) := \sin \theta \int_0^\pi s^{m} \left( \frac{-3h h'}{(1 - h^2)^2} + \frac{(1 + 2h^2) h' a}{(1 - h^2)^{5/2}} \right) \, d\phi
\]
\[
f_4(\theta, \psi) := \sin \theta \int_0^\pi s^{m} \left( \frac{3s^2 h^2 - 4(1 + 2h^2)(h')^2}{(1 - h^2)^3} + \frac{(4(2 + h^2)(h')^2 - s^2(1 + 2h^2)h a}{(1 - h^2)^{7/2}} \right) \, d\phi.
\]
Above, we differentiate under the integral. In Lemma 3.1, we show that for sufficiently high dimension the derivatives with respect to $\psi$ can be interchanged with the integrals over $\theta$ and $\phi$.

**Lemma 3.1.** Using $\tilde{f}_2(\theta, \psi) := \sin \theta \int_0^\pi s^{m-2} \left( \frac{(h')^2}{1 - h^2} + \frac{h s^2 a}{(1 - h^2)^{3/2}} \right) \, d\phi$ we can differentiate under the integral in the following sense, for arbitrary integral bounds of the $\theta$-integral in $[0, \pi]$
\[
\frac{d^2}{d\psi^2} \int \sin \theta \int_0^\pi s^{m-2} a^2 \, d\phi \, d\theta = 2 \int \tilde{f}_2(\theta, \psi) \, d\theta \quad \text{for } m \geq 3 \tag{13}
\]
\[
\frac{d^3}{d\psi^3} \int \sin \theta \int_0^\pi s^{m-2} a^2 \, d\phi \, d\theta = 2 \int \tilde{f}_3(\theta, \psi) \, d\theta \quad \text{for } m \geq 4 \tag{14}
\]
\[
\frac{d^4}{d\psi^4} \int \sin \theta \int_0^\pi s^{m-2} a^2 \, d\phi \, d\theta = 2 \int \tilde{f}_4(\theta, \psi) \, d\theta \quad \text{for } m \geq 5 \tag{15}
\]

**Proof.** For the assertion to hold, it suffices to show, that the $f_j(\theta, \psi)$ are integrable for the respective values of $m$. Since the numerators can all be easily bounded, the only problem is to bound the denominators under the integrals. Recall that $1 - h^2 = (h')^2 + s^2$ and use
\[
\frac{|h'|}{((h')^2 + s^2)^{1/2}} \leq 1 \quad \text{and} \quad \frac{s}{((h')^2 + s^2)^{1/2}} \leq 1 \tag{16}
\]
thus we get

\[
\left| \sin \theta \int_0^\pi s^{m-2} \left( \frac{(h')^2}{1-h^2} + \frac{hs^2a}{(1-h^2)^{3/2}} \right) d\phi \right| \leq (\pi + 1) \sin \theta \int_0^\pi s^{m-3} d\phi \\
\left| \sin \theta \int_0^\pi s^m \left( -3h h' \left( \frac{1}{1-h^2} \right)^2 + \frac{(1+2h^2) h' a}{(1-h^2)^{5/2}} \right) d\phi \right| \leq 3(\pi + 1) \sin \theta \int_0^\pi s^{m-4} d\phi \\
\left| \sin \theta \int_0^\pi s^m \left( \frac{3s^2 h^2 - 4(1+2h^2)(h')^2}{(1-h^2)^3} \right) d\phi \right| \leq 15(\pi + 1) \sin \theta \int_0^\pi s^{m-5} d\phi.
\]

Thus we see that these bounds are finite for the required dimensions. \( \square \)

#### 3.1.3 Rotation Symmetric Measures

Since we restrict attention to rotation symmetric measures, we first calculate \( \tilde{f}_2(\theta,0) \) and \( f_4(\theta,0) \). For the following calculations, note that

\[
h(0,\theta,\phi) = \cos \theta \quad \quad \quad \quad h'(0,\theta,\phi) = \sin \theta \cos \phi \\
a(0,\theta,\phi) := \theta \quad \quad \quad \quad s(\theta,\phi) := \sin \theta \sin \phi.
\]

Using this, we note that

\[
\frac{dF}{d\psi}(\alpha,\beta,0) = \frac{d^3F}{d\psi^3}(\beta,0) = 0.
\]

We use shorthand notation \( I_m := \int_0^\pi \sin^m \phi d\phi \) and we note that \( I_{m-2} = \frac{m}{m-1} I_m \).

\[
\tilde{f}_2(\theta,0) = \sin^{m-1} \theta \int_0^\pi \sin^{m-2} \phi \left( \cos^2 \phi + \frac{\theta \cos \theta \sin^2 \phi}{\sin \theta} \right) d\phi \\
= \sin^{m-1} \theta \left( I_{m-2} - I_m + \frac{\theta \cos \theta}{\sin \theta} I_m \right) = \sin^{m-1} \theta \left( \frac{1}{m-1} \sin \theta + \theta \cos \theta \right) I_m \\
= I_m \frac{1}{m-1} \frac{d}{d\theta} \left( \theta \sin^{m-1} \theta \right).
\]

It is clear that this is positive while \( \frac{1}{m-1} \sin \theta + \theta \cos \theta > 0 \). The point where it switches sign is determined by \( \theta = -\frac{1}{m-1} \tan \theta \), where \( \theta > \pi/2 \). It is clear that for \( m \to \infty \) this point approaches \( \theta = \pi/2 \) from above, as can be seen in Figure 1. More specifically, using \( \theta = \pi/2 + \delta \) and \( 1 - \delta^2/2 \leq \cos \delta \leq 1 - \delta^2/3 \) and \( \delta/2 \leq \sin \delta \leq \delta \), which hold on \([0, \pi/2]\]

\[
\frac{1}{m-1} \sin \theta + \theta \cos \theta < 0 \iff \frac{1}{m-1} \cos \delta - \left( \frac{\pi}{2} - \delta \right) \sin \theta < 0
\]
\[
\iff \frac{1 - \delta^2/3}{m-1} - \left( \frac{\pi}{2} - \delta \right) \delta/2 < 0 \iff \frac{3m - 1}{6(m-1)} \delta^2 - \frac{\pi}{4} \delta + \frac{1}{m-1} < 0
\]
\[
\iff \delta^2 > \frac{6 - 3\pi \delta (m-1)/2}{3m-1} \iff \delta + \frac{\pi}{2} > \theta_{m,4} := \frac{\pi}{2} + \frac{1}{m-1}.
\]
Figure 1: Plots of $\tilde{f}_2(\theta, 0)$, representing the second derivative of the Fréchet function at $\mu$ for a uniformly distributed density on the $S^{m-1}$ at $\theta$ for different dimension $m$. One can clearly see that for $m \to \infty$ the position of the zero approaches $\theta = \pi/2$ from above.

It is clear that for larger $\delta$ than this bound, the contribution to the Hessian is always negative, since the sign cannot change back.

$$f_4(\theta, 0) = \sin^{m-3} \theta \int_0^\pi \sin^m \phi (3 \cos^2 \theta \sin^2 \phi - 4(1 + 2 \cos^2 \theta) \cos^2 \phi) \, d\phi$$

$$+ \sin^{m-4} \theta \int_0^\pi \sin^m \phi \left(4(2 + \cos^2 \theta) \cos^2 \phi - (1 + 2 \cos^2 \theta) \sin^2 \phi\right) \theta \cos \theta \, d\phi$$

$$= \sin^{m-3} \theta \int_0^\pi \sin^m \phi \left(4 + 11 \cos^2 \theta\right) \sin^2 \phi - (4 + 8 \cos^2 \theta) \right) \, d\phi$$

$$+ \sin^{m-4} \theta \int_0^\pi \sin^m \phi \left(- (9 + 6 \cos^2 \theta) \sin^2 \phi + (8 + 4 \cos^2 \theta)\right) \theta \cos \theta \, d\phi$$

$$= I_m \sin^{m-3} \theta \left(\frac{m+1}{m+2} (15 - 11 \sin^2 \theta) - (12 - 8 \sin^2 \theta)\right)$$

$$- I_m \theta \cos \theta \sin^{m-4} \theta \left(\frac{m+1}{m+2} (15 - 6 \sin^2 \theta) - (12 - 4 \sin^2 \theta)\right)$$

$$= \frac{I_m}{m+2} \sin^{m-3} \theta \left((3m - 9) - (3m - 5) \sin^2 \theta\right)$$

$$- \frac{I_m}{m+2} \theta \cos \theta \sin^{m-4} \theta \left((3m - 9) - (2m - 2) \sin^2 \theta\right)$$

$$= \frac{I_m}{m+2} \sin^{m-3} \theta \left((3m - 9) - (3m - 5) \sin^2 \theta\right) - \frac{I_m}{m+2} \theta \frac{d}{d\theta} \left(3 \sin^{m-3} \theta - 2 \sin^{m-1} \theta\right)$$

$$= \frac{I_m}{m+2} \left((3m - 6) \sin^{m-3} \theta - (3m - 3) \sin^{m-1} \theta\right) - \frac{I_m}{m+2} \frac{d}{d\theta} \left(3 \sin^{m-3} \theta - 2 \sin^{m-1} \theta\right).$$

Note that $f_4(\pi/2, 0) = -4$ independent of dimension, as can be seen in Figure 2. We get a condition
for positivity of the fourth derivative, calculated in Appendix A.1.

\[
\theta_{m,4} := \frac{\pi}{2} + \frac{16}{\pi(m-3)}
\]

Figure 2: Plots of \(f_4(\theta,0)\), representing the fourth derivative of the Fréchet function at \(\mu\) for a uniformly distributed density on the \(S^{m-1}\) at \(\theta\) for different dimension \(m\). One can clearly see that for \(m \rightarrow \infty\) the lower bound of the region where the fourth derivative is positive approaches \(\theta = \pi/2\) from above.

It is clear that the above results can be used to describe the behavior of any rotation symmetric measure on \(S^m\). One can also see that there is a region close to \(\theta = 0\), where the second derivative is positive while the fourth derivative is negligible and a region with negative second derivative and positive fourth derivative in the region \(\theta > \pi/2\). Numerically determined values for \(\theta_{m,2}\) and \(\theta_{m,4}\) together with the upper bounds shown above are displayed in Figure 3. This can now be used for explicit calculations on the model described in Equation (12).

Remark 3.2. The fact that both \(\theta_{m,2}\) and \(\theta_{m,4}\) converge to \(\pi/2\) for high dimension with a rate \(m^{-1}\) can be interpreted as follows. There are probability measures for which the Fréchet function has a minimum at the north pole \(\mu = e_{m+1}\) with vanishing Hessian and positive fourth derivative, whose support goes only slightly beyond \(\theta_{m,2}\) and \(\theta_{m,4}\). Consequently, in higher dimension, the measure can be supported on the northern hemisphere and only a small region across the equator in the southern hemisphere and still be smeary. This is an especially egregious example of the curse of dimensionality.
Figure 3: Numerically determined values for $\theta_{m,2}$ and $\theta_{m,4}$ for $m \leq 100$. One can clearly see that the values approach $\pi/2$ from above.

3.1.4 Local Minimum with Vanishing Hessian

In order to achieve a vanishing Hessian at $\mu$, which corresponds to $\psi = 0$, we require

$$0 = \frac{d^2 F}{d\psi^2}(\alpha_0, \beta, 0) = 2(1 - \alpha_0) + 2\alpha_0 g(\beta) \int_{\pi/2}^{\pi - \beta} f_2(\theta, 0) \, d\theta$$

$$= 2(1 - \alpha_0) + 2\alpha_0 I_m g(\beta) \frac{1}{m - 1} \int_{\pi/2}^{\pi - \beta} \frac{d}{d\theta} (\theta \sin^{m-1} \theta) \, d\theta$$

$$= 2(1 - \alpha_0) + 2\alpha_0 I_m g(\beta) \frac{1}{m - 1} \left( (\pi - \beta) \sin^{m-1}(\pi - \beta) - \pi/2 \right).$$

This leads to

$$\frac{1}{1 - \alpha_0} = 1 + \frac{1}{m} \left( \int_{\pi/2}^{\pi - \beta} \sin^{m-1} \theta \, d\theta \right)^{-1} \left( \pi/2 - (\pi - \beta) \sin^{m-1} \beta \right).$$

For a probability measure we have $0 \leq \alpha_0 \leq 1$. Defining the function

$$b_{m,2}(\beta) := \pi/2 - (\pi - \beta) \sin^{m-1} \beta$$

the condition $0 \leq \alpha_0(\beta) \leq 1$ is equivalent to $b_{m,2}(\beta) \geq 0$. Let $\beta_{m,2}$ be the first zero of $b_{m,2}$. To see that $\beta_{m,2} < \pi/2$ note that

$$b_{m,2}(\beta) \leq \frac{\pi}{2} - (\pi - \beta) \left( 1 - \frac{m - 1}{2} \left( \frac{\pi}{2} - \beta \right)^2 \right)$$

$$= -\left( \frac{\pi}{2} - \beta \right) + (\pi - \beta) \left( \frac{m - 1}{2} \left( \frac{\pi}{2} - \beta \right)^2 \right)$$

$$= \frac{m - 1}{2} \left( \frac{\pi}{2} - \beta \right)^3 + \frac{\pi(m - 1)}{4} \left( \frac{\pi}{2} - \beta \right)^2 - \left( \frac{\pi}{2} - \beta \right).$$
Plugging $\beta = \frac{\pi}{2} - \frac{1}{2(m-1)}$ into the right hand side, we get for $m \geq 2$

$$b_{m,2} \left( \frac{\pi}{2} - \frac{1}{2(m-1)} \right) \leq \frac{1 - (8 - \pi)(m-1)}{16(m-1)^2} \leq 0 \quad \Rightarrow \quad \beta_{m,2} \leq \frac{\pi}{2} - \frac{1}{2(m-1)}.$$ 

Furthermore, note that using $\delta = \frac{\pi}{2} - \beta$,

$$b_{m,2} = \frac{\pi}{2} - \left( \frac{\pi}{2} + \delta \right) \cos^{m-1} \delta \geq 0$$

$$\Leftrightarrow \cos \delta \leq \left(1 + \frac{2\delta}{\pi} \right)^{-\frac{1}{m-1}} = 1 - \frac{\delta^2}{3} \leq 1 - \frac{2\delta}{\pi(m-1)} \quad \Leftrightarrow \quad \delta \leq \frac{6}{\pi(m-1)}$$

and therefore

$$\beta_{m,2} \geq \frac{\pi}{2} - \frac{6}{\pi(m-1)}.$$ 

Using the upper bound for $\beta$, we can derive a lower bound for $\alpha_0$, which is stronger than $\alpha_0 \geq 0$, namely

$$1/\alpha_0 \leq 1 + \frac{\pi}{2m} \left( \int_{\pi/2}^{\pi + \frac{1}{3}} \sin^{m-1} \theta \, d\theta \right)^{-1}$$

$$\leq 1 + \frac{\pi}{2m} \left( \int_0^{1/m} \left( 1 - \frac{m-1}{2} \theta^2 \right) \, d\theta \right)^{-1}$$

$$= 1 + \frac{3\pi(m-1)^2}{m(6(m-1)-1)}.$$ 

In summary, an $\alpha_0$, such that the Hessian vanishes, exists for $(\pi/2 - (\pi - \beta) \sin^{m-1} \beta) > 0$, which can indeed be satisfied, as evidenced by the lower bound $\beta_{m,2}$ determined here. Note that this result is valid for all $m \geq 3$.

However, the fourth derivative can only be determined for $m \geq 5$. We have

$$\frac{d^4 F}{d\psi^4}(\alpha_0, \beta, 0) = 2\alpha_0 g(\beta) \int_{\pi/2}^{\pi - \beta} f_4(\theta, 0) \, d\theta$$

$$= 2\alpha_0 I_m g(\beta) \int_{\pi/2}^{\pi - \beta} \sin^{m-3} \theta \left( (3m - 6) - (3m - 3) \sin^2 \theta \right) \, d\theta$$

$$- 2\alpha_0 I_m g(\beta) \int_{\pi/2}^{\pi - \beta} \frac{d}{d\theta} \left( 3\theta \sin^{m-3} \theta - 2\theta \sin^{m-1} \theta \right) \, d\theta$$

$$= 2\alpha_0 I_m g(\beta) \int_{\pi/2}^{\pi - \beta} \left( (3m - 6) \sin^{m-3} \theta - (3m - 3) \sin^{m-1} \theta \right) \, d\theta$$

$$+ 2\alpha_0 I_m g(\beta) \left( \pi - (\pi - \beta) \left( 3 \sin^{m-3} (\pi - \beta) - 2 \sin^{m-1} (\pi - \beta) \right) \right)$$

$$= 2\alpha_0 I_m g(\beta) \left( 3 \sin^{m-2} \beta \cos (\pi - \beta) - 3(\pi - \beta) \sin^{m-3} \beta + 2(\pi - \beta) \sin^{m-1} \beta + \frac{\pi}{2} \right).$$

Using

$$b_{m,4}(\beta) := \frac{\pi}{2} + 2(\pi - \beta) \sin^{m-1} \beta - 3 \cos \beta \sin^{m-2} \beta - 3(\pi - \beta) \sin^{m-3} \beta$$

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we can give the necessary condition \( b_{m,4}(\beta) > 0 \) for a local minimum of the Fréchet function at \( \psi = 0 \). From this relation we can determine a minimal \( \beta_{m,4} \) such that \( b_{m,4}(\beta_{m,4}) \geq 0 \) for every dimension \( m \geq 4 \) giving a dimension dependent maximal hole size. Note that

\[
\begin{align*}
\left( b_{m,2}(\beta) - b_{m,4}(\beta) \right) &= -3(\pi - \beta) \sin^{m-1} \beta + 3 \cos \beta \sin^{m-2} \beta + 3(\pi - \beta) \sin^{m-3} \beta \\
&= 3 \cos \beta \sin^{m-2} \beta + 3(\pi - \beta) \cos^2 \beta \sin^{m-3} \beta \geq 0,
\end{align*}
\]

which implies \( \beta_{m,4} \leq \beta_{m,2} \).

Furthermore, we calculate in Appendix A.2

\[
b_{m,4}(\beta) \leq -\frac{5 + \pi}{2} \left( \frac{\pi}{2} - \beta \right) + \frac{\pi(m - 3)}{4} \left( \frac{\pi}{2} - \beta \right)^2 + \frac{(5 + \pi)(m - 3) + 3}{4} \left( \frac{\pi}{2} - \beta \right)^3
\]

which leads to the upper bound

\[
\beta_{m,4} \leq \frac{\pi}{2} - \frac{1}{m - 3}.
\]

Analogously, we can calculate in Appendix A.2 the lower bound

\[
\beta_{m,4} \geq \frac{\pi}{2} - \frac{6(6 + \pi)}{\pi(m - 3)}.
\]

As a result, both \( \beta_{m,2} \) and \( \beta_{m,4} \) converge to \( \frac{\pi}{2} \) with order \( \frac{1}{m} \) as \( m \to \infty \).

Figure 4: Numerically determined values for \( \beta_{m,2} \) and \( \beta_{m,4} \) for \( m \leq 100 \). One can clearly see that the values approach \( \pi/2 \) from below.

**Remark 3.3.** As pointed out before in Remark 3.2, the fact that both \( \beta_{m,2} \) and \( \beta_{m,4} \) converge to \( \pi/2 \) for high dimension with a rate \( m^{-1} \) displays the curse of dimensionality. There are probability measures for which the Fréchet function has a minimum at the north pole \( \mu = e_2 \) with vanishing Hessian and positive fourth derivative, whose support only contains a small region close to the equator in the southern hemisphere.
3.1.5 Global Minimum

To show that the local minimum at $\psi = 0$ is indeed a global minimum at least for some $\beta > 0$, we use a Lipschitz argument as follows. Recall that for $\beta = 0$

$$\forall \psi \in (0, \pi] : \frac{d^2 F}{d\psi^2} > 0 \quad \forall \psi \in (0, \pi) : \frac{d^4 F}{d\psi^4} > 0 \quad \forall \psi \in [0, \pi/2) : \frac{d^5 F}{d\psi^5} > 0.$$ 

To show that we have a global minimum at $\psi = 0$, we need $\forall \psi \in (0, \pi] : \frac{d^5 F}{d\psi^5} > 0$. In order to show this, we prove the following Lipschitz conditions, where $\alpha_i$ denotes the $\alpha_0$ corresponding to $\beta_i$.

Lemma 3.4.

$$\left| \frac{d^3F}{d\psi^3}(\alpha_1, \beta_1, \psi) - \frac{d^3F}{d\psi^3}(\alpha_2, \beta_2, \psi) \right| \leq L_2|\beta_1 - \beta_2| \quad (18)$$

$$\left| \frac{d^3F}{d\psi^3}(\alpha_1, \beta_1, \psi) - \frac{d^3F}{d\psi^3}(\alpha_2, \beta_2, \psi) \right| \leq L_3|\beta_1 - \beta_2| \quad (19)$$

$$\left| \frac{d^4F}{d\psi^4}(\alpha_1, \beta_1, \psi) - \frac{d^4F}{d\psi^4}(\alpha_2, \beta_2, \psi) \right| \leq L_4|\beta_1 - \beta_2| \quad (20)$$

Proof. Note that

$$L_k \geq \max_{\beta \in [0, \beta_{m, 4}], \psi \in [0, \pi]} \left| \frac{d^3F}{d\beta d\psi^2}(\alpha, \beta, \psi) \right|$$

are valid Lipschitz constants. Thus we note for $j = 2, 3, 4$

$$\frac{d^{j+1}F}{d\beta d\psi^j} = \frac{d}{d\beta} \left( \alpha(\beta) g(\beta) \int_{\pi/2}^{\pi-\beta} f_j(\theta, \psi) d\theta \right)$$

$$= 2g \frac{d\alpha}{d\beta} \int_{\pi/2}^{\pi-\beta} f_j(\theta, \psi) d\theta + 2\alpha g \frac{dg}{d\beta} \int_{\pi/2}^{\pi-\beta} f_j(\theta, \psi) d\theta - 2\alpha g f_j(\pi - \beta, \psi)$$

We know $|\alpha| = \alpha < 1$ and $|g| = g \leq g(0)$. $\left| \frac{d\alpha}{d\beta} \right|$ and $\left| \frac{dg}{d\beta} \right|$ can also trivially be bounded, since $\beta_{m, 4} < \pi/2$. So only $f_j(\theta, \psi)$ and their $\theta$ integrals remain to be bounded. Since the numerators can all be easily bounded, the only problem is to bound the denominators under the integrals. Using the boundedness shown in Lemma 3.1 we see that we need $m \geq 5$ for these bounds to be finite.

Collecting all the estimates, we get the desired Lipschitz constants. \qed

Using the Lipschitz constants, we can now show that the local minima are global for suitably small $\beta > 0$.

Remark 3.5. Note that the estimates in Equation (16) are very generous and might be improved by a more careful treatment. Therefore, the fact that the result of Lemma 3.4 only hold for dimension $m \geq 5$ should not be seen as a fundamental restriction.

Theorem 3.6. For $m \geq 5$ there is a $\beta_0 > 0$ such that the measure the model described in Equation (12) has a unique 2-smeary Fréchet mean with asymptotic rate $n^{-1/6}$ at the north pole for any $\beta \leq \beta_0$.

Proof. We recall $\frac{d^2F}{d\psi^2}(\alpha_0, 0, 0) = 2\frac{m+1}{m} - 1 = \epsilon_m > 0$ and that the inequality is (8) is strict for $\delta \neq 0, \pi$, due to $0 < h(\theta) < 1$ for all $\theta \in (-\pi/2, \pi/2)$ for $m^{-1}$. Hence we infer that $G'(\delta)$ is strictly increasing in $\delta$ from $G'(0) = 0$, yielding that there is no stationary point for $F$ other than $p = \mu$.

Due to Equation (11) we know for all $\psi \leq \pi/3$

$$\frac{d^4F}{d\psi^4}(\alpha, \beta, \psi) \geq \frac{d^4F}{d\psi^4}(\alpha_0, 0, \psi) - L_4\beta \geq \frac{\epsilon_m}{2} - \frac{L_4}{2}$$

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Thus we can pick $\beta \leq \frac{c_m}{2L_4}$ to get $\frac{d^2F}{d\psi^2}(\alpha_\beta, \beta, \psi) \geq 0$ for all $\psi \leq \pi/3$. Since $\frac{d^2F}{d\psi^2}(\alpha_\beta, 0, 0) = 0$ and $\frac{d^2F}{d\psi^2}(\alpha_\beta, \beta, 0) = 0$ it follows that $\frac{d^2F}{d\psi^2}(\alpha_\beta, \beta, \psi) > 0$ and $\frac{d^2F}{d\psi^2}(\alpha_\beta, \beta, \psi) > 0$ for all $0 < \psi \leq \pi/3$.

From Equation (18) we note that

$$\left| \frac{d^2F}{d\psi^2}(\alpha_0, \beta, \psi) - \frac{d^2F}{d\psi^2}(\alpha_\beta, \beta, \psi) \right| \leq L_2|\beta|.$$ 

Thus we can pick $\beta < \frac{1}{L_2} \frac{d^2F}{d\psi^2}(\alpha_0, 0, \pi/3)$ to achieve $\frac{d^2F}{d\psi^2}(\alpha_\beta, \beta, \pi/3) \geq \frac{d^2F}{d\psi^2}(\alpha_0, 0, \pi/3) - L_2\beta > 0$. Since $\frac{d^2F}{d\psi^2}(\alpha_0, 0, \psi)$ is monotonously growing in $\psi$, it follows that $\frac{d^2F}{d\psi^2}(\alpha_\beta, \beta, \psi) > 0$ for all $\psi \geq \pi/3$. Thus for all $\beta < \beta_0 = \min \left( \frac{c_m}{2L_4}, \frac{1}{L_2} \frac{d^2F}{d\psi^2}(\alpha_0, 0, \pi/3) \right)$ (21)

the minimum at $\psi = 0$ is unique. $\square$

Theorem 3.6 shows that it is not necessary that the probability density assumes a specific critical value at the cut locus in order to cause smeariness. This is in stark contrast to the situation on the circle, see Hotz and Huckemann (2015). In fact, smeariness can even occur, if a neighborhood around the cut locus does not contain any probability mass. This means that the manifold can be deformed to eliminate the cut locus altogether. More precisely, specific topological properties are not needed for the Fréchet mean to have a smeary asymptotic rate. Instead, the basis for smeariness in the case of higher dimensional spheres appears to be geometrical.

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A Technical Calculations and Proofs

A.1 Calculation of Bound for $\theta_{m, \delta}$

To get a lower bound on the region of positive fourth derivative, we write again $\theta = \pi/2 + \delta$ and define

$$f(\delta) = \left( (3m - 9) - (3m - 5) \cos^2 \delta \right) \cos \delta + \left( (3m - 9) - (2m - 2) \cos^2 \delta \right) \left( \frac{\pi}{2} + \delta \right) \sin \delta .$$

We can immediately see

$$f(\delta) \geq (3m - 9) + \frac{\pi}{2} (3m - 9) \sin \delta - (3m - 5) \cos^3 \delta - (2m - 2) \left( \frac{\pi}{2} + \delta \right) \sin \delta \cos^2 \delta$$

$$\geq (3m - 9) + \frac{\pi}{2} (3m - 7) \sin \delta - (3m - 5) \cos^3 \delta - (2m - 2) \delta \sin \delta \cos^2 \delta$$

$$\geq (3m - 9) + \frac{\pi}{4} (3m - 7) \delta - (3m - 5) \cos^3 \delta - (2m - 2) \delta \sin \delta \cos^2 \delta .$$

**Lemma A.1.** To bound the remaining trigonometric function terms, we show by induction over $m$ that

$$g_m(\delta) := (3m - 5) \cos^3 \delta + (2m - 2) \delta \sin \delta \cos^2 \delta \leq (3m - 5) - (m - 3)\delta^2 .$$

**Proof.** For $m = 2$, the inequality reads

$$g_2(\delta) = \cos^3 \delta + 2\delta \sin \delta \cos^2 \delta \leq 1 + \delta^2 .$$
Inserting $\delta = 0$ the inequality holds. Now consider the derivative
\[
g'_2(\delta) = 2\delta \cos \delta - \sin \delta \cos^2 \delta - 6\delta \sin^2 \delta \cos \delta \leq 2\delta,
\]
which is obviously true and thus proves the claim for $m = 2$.
For the induction step, we must show
\[
g_0(\delta) := 3 \cos^3 \delta + 2\delta \sin \delta \cos^2 \delta \leq 3 - \delta^2.
\]
First, note that
\[
3 \cos \delta + 2\delta \sin \delta \leq 3 + \frac{\delta^2}{2}
\]
\[
- \sin \delta + 2\delta \cos \delta \leq \delta
\]
\[
\cos \delta - 2\delta \sin \delta \leq 1
\]
where the left inequalities reflect the values for $\delta = 0$ and we perform derivatives from row to row. Next we note
\[
3 \cos^2 \delta + \frac{\delta^2}{2} \cos^2 \delta \leq 3 \cos^2 \delta + \frac{1}{2} \sin^2 \delta
\]
\[
\iff \delta \cos \delta \leq \sin \delta.
\]
This last estimate has the important property that its second derivative is monotonically growing on $[0, \pi/2]$. Therefore, once $3 \cos^2 \delta + \frac{1}{2} \sin^2 \delta > 3 - \delta^2$ for some delta, it would also hold for all larger $\delta$, particularly $\delta = \pi/2$. Since
\[
\frac{1}{2} \leq 3 - \frac{\pi^2}{4}
\]
we have finally shown $g_0(\delta) \leq 3 - \delta^2$ as desired.

Thus we can write
\[
f(\delta) \geq (3m - 9) + \frac{\pi(m-7)}{4} \delta - (3m - 5) + (m - 3)\delta^2.
\]
and plugging in $\theta_{m,4} - \pi/2 = \frac{16}{\pi(m-3)}$, we get
\[
f(\theta_{m,4} - \pi/2) \geq -4(m - 3) + 4(m - 7) + \frac{256}{\pi^2} = \frac{256}{\pi^2} - 16 > 0.
\]

A.2 Calculation of Bounds for $b_{m,4}$ and $\beta_{m,4}$

Let $\delta = \frac{\pi}{2} - \beta$ and use $1 - \delta^2/2 \leq \cos \delta \leq 1 - \delta^2/3$ and $\delta/2 \leq \sin \delta \leq \delta$, which hold on $[0, \pi/2]$, then, assuming $m \geq 3$
\[
b_{m,4}(\beta) = \frac{\pi}{2} + 2(\pi - \beta) \sin^{m-1} \beta - 3 \cos \beta \sin^{m-2} \beta - 3(\pi - \beta) \sin^{m-3} \beta
\]
\[
= \frac{\pi}{2} + 2 \left( \frac{\pi}{2} + \delta \right) \cos^{m-1} \delta - 3 \sin \delta \cos^{m-2} \delta - 3 \left( \frac{\pi}{2} + \delta \right) \cos^{m-3} \delta
\]
\[
= \frac{\pi}{2} - (1 + 2 \sin^2 \delta) \left( \frac{\pi}{2} + \delta \right) \cos^{m-3} \delta - 3 \sin \delta \cos^{m-2} \delta
\]
\[
\leq \frac{\pi}{2} - \left( \frac{\pi}{2} + \delta \right) \left( 1 - \frac{m-3}{2} \delta^2 \right) - \frac{3}{2} \delta \left( 1 - \frac{m-2}{2} \delta^2 \right)
\]
\[
= \frac{5}{2} \delta + \frac{\pi(m-3)}{4} \delta^2 + \frac{5(m-3)}{4} + 3 \delta^3.
\]
Now, plugging in $\delta = \frac{1}{2(m-3)}$, we get for $m \geq 4$
\[
b_{m,4}(\beta) \leq -\frac{5}{4(m-3)} + \frac{\pi}{16(m-3)} + \frac{(5 + \pi)(m - 3) + 3}{32(m - 3)^3} = \frac{(-40 + 2\pi)(m - 3)^2 + (5 + \pi)(m - 3) + 3}{32(m - 3)^3} \leq 0.
\]
From this, we get the upper bound
\[
\beta_{m,4} \leq \frac{\pi}{2} - \frac{1}{2(m-3)}.
\]

Analogously, we show the lower bound, by first noting
\[
b_{m,4}(\beta) = \frac{\pi}{2} - (1 + 2\sin^2{\delta}) \left(\frac{\pi}{2} + \delta\right) \cos^{m-3} \delta - 3\sin \delta \cos^{m-2} \delta
\]
\[
= \frac{\pi}{2} - (\frac{\pi}{2} + \delta + 2\delta \sin^2{\delta} + \pi \sin^2{\delta} + 3\sin \delta \cos \delta) \cos^{m-3} \delta
\]
\[
\geq \frac{\pi}{2} - (\frac{\pi}{2} + (6 + \pi)\delta) \cos^{m-3} \delta
\]
and then calculating
\[
b_{m,4} = \frac{\pi}{2} - (\frac{\pi}{2} + (6 + \pi)\delta) \cos^{m-3} \delta \geq 0
\]
\[
\Leftrightarrow \cos \delta \leq \left(1 + \frac{2(6 + \pi)\delta}{\pi}\right)^{-\frac{1}{m-3}} \Leftrightarrow 1 - \frac{\delta^2}{3} \leq 1 - \frac{2(6 + \pi)\delta}{\pi(m-3)} \Leftrightarrow \delta \leq \frac{6(6 + \pi)}{\pi(m-3)}
\]
which establishes the lower bound
\[
\beta_{m,4} \geq \frac{\pi}{2} - \frac{6(6 + \pi)}{\pi(m-3)}.
\]

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