Behavior of Fréchet mean and Central Limit Theorems on spheres
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Abstract

Jacobi fields are used to compute higher derivatives of the Fréchet function on spheres with absolutely continuous rotationally symmetric probability distribution. Consequences include (i) a practical condition to test if the mode of the symmetric distribution is a local Fréchet mean; (ii) a Central Limit Theorem on spheres with practical assumptions and an explicit limiting distribution; and (iii) an answer to the question of whether the smeary effect can occur on spheres with absolutely continuous and rotationally symmetric distributions: with the method presented here, it can in dimension at least 4.

Keywords: Spherical statistic, Fréchet mean, central limit theorem, smeary
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1 Introduction

Methods of deriving Central Limit Theorems (CLT) for intrinsic Fréchet means on manifolds in [BP05, HH15, BL17, EH18] often rely on Taylor expansion of the Fréchet function at the mean. Thus, two scenarios can happen depending on the invertibility of the Hessian of the Fréchet function. The first case, in which the Hessian is invertible and positive definite, results in a CLT that behaves classically as shown in [BL17]. The other one, when the Hessian vanishes at the mean, results in a non classical behavior called smeary CLT as first shown in [HH15, EH18]. In both cases, an assumption about the differentiability the Fréchet function in a neighborhood of the mean is required. Otherwise, the reference measure would be required to give no mass to an open neighborhood of the cut locus of the mean [EGH+19]. The reason for this assumption is that the squared distance function from a point is not differentiable at its cut locus, which means that the derivative tensors would blow up near the cut locus.

This problem is addressed here by giving a practical condition to test if the Fréchet function is differentiable at a point on a sphere of arbitrary dimension (Proposition 3.1). Specifically, the central observation is that in dimension at least 4 the Fréchet function has derivative of order 4 at a point $p$ if the reference measure has a bounded distribution

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function (with respect to the volume measure) in an open neighborhood of the antipode of \( p \).

In the classical CLT case on manifolds, an assumption about the invertibility of the Hessian of the Fréchet function at the mean is also required. The CLTs by [BL17] and [EH18] give general forms, which need explicitly computed derivatives of the Fréchet function to be made precise. To date, a CLT with an explicit limit distribution for Fréchet means is only available on circles [HH15] and on spheres with a specific model considered in [EH18].

Here we fill this gap, for the case of absolutely continuous and rotationally symmetric distributions on spheres, by giving an explicit sufficient condition for the Hessian to be positive definite, along with an explicit limit distribution for the CLT. In particular, the assumption that the measure is absolutely continuous and rotationally symmetric about a point \( p \) allows the computation of the derivative tensors of the Fréchet function at its mean. Two consequences include a practical condition for \( p \) to be a local Fréchet mean (Proposition 4.1) and a Central Limit Theorem with an explicit limit distribution with Fréchet mean at \( p \) (Theorem 5.1).

Section 5 studies the smeary version of the CLT for absolutely continuous and rotationally symmetric distributions on spheres. The smeary effect occurs when the Hessian of the Fréchet function vanishes and a tensor obtained by differentiating an even number of times is positive definite at the Fréchet mean. In those cases, the sample mean fluctuates asymptotically at a scale of \( n^{\alpha} \) for some \( \alpha < 1/2 \). To date, examples of smeary CLT on circles and spheres were observed in [HH15, EH18, Elt19]. In those examples, the reference measures are singular at the mean. A natural question arises: can smeariness happen for non-singular measures?

The computation of derivative tensors yields an answer to this question on spheres, when the distribution is rotationally symmetric. In particular, in that setup when the distribution is absolutely continuous, under a minimal assumption (Proposition 3.1), the smeary effect can only appear in dimension 4 or higher and is more likely as the dimension grows (Remark 5.7). This is because of the fact that in low dimension, the volume element cannot outweigh the negativity of the derivative tensor at the cut locus of the mean. As a result, the derivative tensor of order 4 is always negative in dimension 2 and 3. In higher dimension, we give a sufficient condition for a smeary CLT to occur with \( \alpha = 1/6 \) (Theorem 5.4).

The first example of a smeary CLT on spheres with no mass in a neighborhood of the cut locus of the mean was shown in [EH19]. In that example, the reference measure gives a singular mass to the mean. Example 5.6 exhibits the smeary effect of a local Fréchet mean when the measure has no singular mass. Specifically, the measure has a uniformly distributed portion on a bottom cup and another uniformly distributed portion on a thin upper strip near the equator and zero everywhere else. The South pole is a local mean and the strip near the equator gets thinner as the dimension grows.

In contrast to the method of expressing the Fréchet function explicitly in a polar coordinate system as shown in [HH15, EH18, Elt19], the main method used in this paper is applying Jacobi fields with a non-parametric approach to compute derivative tensors of the squared distance function on spheres (Section 2). The rotationally symmetric condition of the distribution then allows us to derive derivative tensors of the Fréchet function (Section 3). This method of applying Jacobi fields with a non-parametric ap-
approach to derive derivatives of squared distance function could be applied to symmetric spaces since Jacobi fields in such spaces can be explicitly expressed. However, behaviors of Frechét mean on symmetric spaces still remains unknown because derivatives of the squared distance function do not translate well to corresponding derivatives of Frechét function as it is in the case on spheres. Obstacles include (i) the cut locus of a point can be a closed set rather than a single point; and (ii) it is difficult to generalize a notion of rotationally symmetric on symmetric spaces. Thus, further research is required for symmetric spaces and homogeneous spaces in general.

It is also worth mentioning that the method in this paper does not work well for models in spheres of dimension 2 and 3 in which there is a singular mass at the cut locus of the mean. In such scenarios, writing the Frechét function explicitly in a coordinate system yields better results, as shown in [EH18].

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2 Derivative tensors of the squared distance function

In this section, the second order derivative tensor of the squared distance function is computed (c.f. 2.1). The results are used to compute the third and the fourth derivative of the squared distance function (c.f. 2.5, 2.9).

2.1 The second derivative

Consider the $d$-dimensional unit sphere $S^d$, $d \geq 2$ with geodesic distance $d$ and Riemannian metric $g$. Fix a point $y$ in $S^d$, define

$$h_y(p) := \frac{1}{2} d^2(y, x) = \frac{1}{2} d_y^2(x).$$

Call $C_y$ the cut locus of $y$, which in this case is its antipode. It is well known that $h_y(x)$ is differentiable on $S^d \setminus C_y$. In this section, we will compute the second derivative tensor $\nabla^2 h_y$ of $h_y$ at a point $x \neq C_y$.

Let $\mathfrak{X}(S^d)$ and $\mathcal{D}(S^d)$ be the space of vector fields and the space of real valued functions on $S^d$ that are of class $C^\infty$ on $S^d \setminus C_y$, respectively. Let $Y$ denote the vector field $\nabla h_y$, then for any point $x$ the vector $(-Y(x)) \in T_x S^n$ is the tangent vector of the geodesics (parametrized by arc length) connecting $x$ and $y$. Recall that the Hessian operator $\nabla^2 h_y$ at $x$ is a linear map $\nabla^2 h_y(x) : T_x M \to T_x M$ defined by the following identity

$$\nabla^2 h_y \cdot v = \nabla_v (\nabla h_y) = \nabla_v Y = \nabla_x Y(x),$$

3
where \( v \in T_x M \), \( Z \) is a vector field in \( S^d \) with \( Z(x) = v \) and \( \nabla_Z \) stands for the covariant derivative in direction \( Z \). We wish to compute \( \nabla_Z Y \) for any vector field \( Z \in \mathcal{X}(S^d) \). If there is no confusion arise, we will write \( \langle Y, Z \rangle \) for \( g(Y, Z) \) and \( \|Y\| \) for \( \|Y(x)\| \).

Let \( \gamma(t) \) and \( \eta(s) \) be the geodesics parametrized by arc length that start at \( (-Y(0), 0) \) and \( Z(x) \), respectively. Consider the following smooth parametered surface

\[
 f : [0, 1]^2 \to M \\
 (s, t) \mapsto \exp_{\gamma(s)} \left(-tY(\eta(s))\right).
\]

Taking derivatives of \( f \) in \( s \) and \( t \) gives

\[
 D_s \frac{d}{dt} f(t, s) = D_t \frac{d}{ds} f(s, t).
\]

Note that \( D_s \frac{d}{dt} f(t, s) = -D_s \nabla h_y(\eta(s)) \) and \( D_t \frac{d}{ds} f(s, t) |_{s=0} = \nabla_Z Y(x) \), so

\[
 \nabla_Z Y(x) = -\frac{D}{Dt} \frac{d}{ds} f(s, t) |_{(0, 0)}.
\]

Observe that the vector field

\[
 J(t) := \frac{d}{ds} f(s, t) |_{s=0}
\]

is a Jacobi field along \( \gamma(t) \) with \( J(0) = Z(x), \ J(1) = 0 \) ([Car12], Chap. 5, Cor. 2.5.,) then

\[
 \nabla_Z Y(x) = J'(0) = \frac{D}{Dt} J(t) |_{t=0}.
\]

Call \( P_T \) and \( P^\perp \) the projection on \( Y(x) \) and \( Y(x)^\perp \) respectively. Also let \( J^T(t) \) and \( J^\perp(t) \) be the Jacobi field along \( \gamma(t) \) with

\[
 J^T(1) = J^\perp(1) = 0,
\]

and

\[
 J^T(0) = P_T(Z(x)), \ J^\perp(0) = P^\perp(Z(x))
\]

then

\[
 J = J^T + J^\perp.
\]

Since \( S^d \) has constant sectional curvature, we can write the equation of \( J^T \) and \( J^\perp \) explicitly as

\[
 J^T(t) = (1-t) P_T(Z(x)),
\]

\[
 J^\perp(t) = -P^\perp(Z(x)) \left( \cot(||Y||) \sin(t||Y||) - \cos(t||Y||) \right).
\]

Therefore

\[
 J'(0) = (J^T)'(0) + (J^\perp)'(0)
\]

\[
 = -P_T(Z(x)) - ||Y|| \cot(||Y||) P^\perp(Z(x))
\]

\[
 = Z||Y|| \cot(||Y||) - Y^2 \frac{\langle Y, Z \rangle}{||Y||^2} \left( ||Y|| \cot(||Y||) - 1 \right).
\]

4
Thus, we have the result for the second derivative tensor of $h_y$

$$\nabla^2 h_y(Z) = \nabla_Z Y = Z\|Y\| \cot(\|Y\|) - Y \frac{\langle Y, Z \rangle}{\|Y\|^2} \left(\|Y\| \cot(\|Y\|) - 1\right). \quad (2.1)$$

### 2.2 Higher order derivatives

Following notations of derivative tensors in Sec. 5, Chap. 4, [Car92], we view $\nabla^2 h_y$ as a 2-tensor. It follows from (2.1) that

$$\nabla^2 h_y(Z, T) = \nabla Y(Z, T)$$

$$= Z\langle Y, T \rangle - \langle Y, \nabla_Z T \rangle$$

$$= \langle Z, T \rangle \|Y\| \cot(\|Y\|) - \langle Y, T \rangle \frac{\langle Y, Z \rangle}{\|Y\|^2} \left(\|Y\| \cot(\|Y\|) - 1\right),$$

for any vector fields $Z, T \in \mathcal{X}(S^d)$. Here recall that we write $\|Y\|$ and $\|Y\| \cot(\|Y\|)$ for $\|Y(x)\|$ and $\|Y(x)\| \cot (\|Y(x)\|)$, respectively. For later use, we define

$$g_y : S^d \rightarrow \mathbb{R}$$

$$x \mapsto \|Y(x)\| \cot (\|Y(x)\|) = \|Y\| \cot (\|Y\|),$$

and rewrite the tensor $\nabla^2 h_y$ as

$$\nabla^2 h_y(Z, T) = \langle \nabla_Z Y, T \rangle = \langle Z, T \rangle g_y - \langle Y, T \rangle \frac{\langle Y, Z \rangle}{\|Y\|^2} \left(g_y - 1\right). \quad (2.2)$$

Using (2.1), the gradient of $g$ can be computed as

$$\nabla g_y = \frac{Y}{\|Y\|^2} g_y' \quad \text{where } g_y' \text{ is the formal derivative of } g_y$$

$$g_y' = \cot(\|Y\|) - \|Y\| \frac{\|Y\|}{\sin^2(\|Y\|)}.$$ 

Using the identity

$$\frac{d}{dt} t \cot t = t \cot t - (t \cot t)^2 - t^2$$

we have

$$\|Y\| g_y' = g_y - g_y^2 - \|Y\|^2.$$ 

Thus, (2.3) can be rewritten as

$$\nabla g_y = \frac{Y}{\|Y\|^2} \left(g_y - g_y^2 - \|Y\|^2\right). \quad (2.4)$$
Using (2.2) and (2.4), the third derivative $\nabla^3 h_y$ can be computed formally as
\[ \nabla^3 h_y(W, Z, T) = W(\nabla^2 h_y(Z, T)) - \nabla^2 h_y(\nabla W Z, T) - \nabla^2 h_y(Z, \nabla W T) \]
\[ = (\langle Z, T \rangle \langle Y, W \rangle + \langle W, T \rangle \langle Y, Z \rangle + \langle W, Z \rangle \langle Y, T \rangle) \frac{g_y - g_y^2}{\|Y\|^2} + \langle Y, W \rangle \langle Y, Z \rangle \frac{3g_y^2 - 3g_y + \|Y\|^2}{\|Y\|^4} - \langle Z, T \rangle \langle Y, W \rangle. \tag{2.5} \]

In a similar manner, the fourth derivative tensor is the following 4-tensor
\[ \nabla^4 h_y(U, W, Z, T) = U(\nabla^3 h_y(W, Z, T)) - \nabla^3 h_y(\nabla_U W, Z, T) - \nabla^3 h_y(W, \nabla_U Z, T) - \nabla^3 h_y(W, Z, \nabla U T). \]
To simplify notations, let us introduce
\[ \Sigma_1 := (\langle Z, T \rangle \langle Y, W \rangle + \langle W, T \rangle \langle Y, Z \rangle + \langle W, Z \rangle \langle Y, T \rangle), \]
\[ \Sigma_1' := (\langle Z, T \rangle \langle \nabla_U Y, W \rangle + \langle W, T \rangle \langle \nabla_U Y, Z \rangle + \langle W, Z \rangle \langle \nabla_U Y, T \rangle), \]
\[ \Sigma_2 := \langle Y, W \rangle \langle Y, Z \rangle \langle Y, T \rangle, \]
\[ \Sigma_2' := \langle \nabla_U Y, W \rangle \langle Y, Z \rangle \langle Y, T \rangle + \langle Y, W \rangle \langle \nabla_U Y, Z \rangle \langle Y, T \rangle + \langle Y, W \rangle \langle Y, Z \rangle \langle \nabla_U Y, T \rangle. \]

Then
\[ \nabla^4 h_y(U, W, Z, T) = \Sigma_1 \frac{g_y - g_y^2}{\|Y\|^2} + \Sigma_1 U \left( \frac{g_y - g_y^2}{\|Y\|^2} \right) \]
\[ + \Sigma_2 \frac{3g_y^2 - 3g_y + \|Y\|^2}{\|Y\|^4} + \Sigma_2 U \left( \frac{3g_y^2 - 3g_y + \|Y\|^2}{\|Y\|^4} \right) - \langle Z, T \rangle \langle \nabla_U Y, W \rangle. \tag{2.6} \]

Identities (2.2) and (2.4) give us explicit expression of $\Sigma_1'$ and $\Sigma_2'$
\[ \Sigma_1' = (\langle Z, T \rangle \langle U, W \rangle + \langle W, Z \rangle \langle U, T \rangle + \langle W, T \rangle \langle U, Z \rangle) g_y \]
\[ + \frac{1 - g_y}{\|Y\|^2} \left( \langle Y, U \rangle \langle Y, W \rangle \langle Z, T \rangle + \langle Y, U \rangle \langle Y, Z \rangle \langle W, T \rangle + \langle Y, U \rangle \langle Y, T \rangle \langle Z, W \rangle \right), \]
\[ \Sigma_2' = (\langle U, W \rangle \langle Y, Z \rangle \langle Y, T \rangle + \langle U, Z \rangle \langle Y, W \rangle \langle Y, T \rangle + \langle U, T \rangle \langle Y, Z \rangle \langle Y, W \rangle) g_y \]
\[ + 3 \langle Y, U \rangle \langle Y, W \rangle \langle Y, Z \rangle \langle Y, T \rangle \frac{1 - g_y}{\|Y\|^2}, \]
and
\[ U \left( \frac{g_y - g_y^2}{\|Y\|^2} \right) = \frac{\langle Y, U \rangle}{\|Y\|^4} \left( \frac{2g_y^3 - g_y^2 - g_y + \|Y\|^2 + 2\|Y\|^2 g_y}{\|Y\|^2} \right). \tag{2.7} \]

To further simplify our notations, set
\[ I_1 := \langle Z, T \rangle \langle U, W \rangle + \langle W, Z \rangle \langle U, T \rangle + \langle W, T \rangle \langle U, Z \rangle, \]
\[ I_2 := \langle Y, U \rangle \langle Y, W \rangle \langle Z, T \rangle + \langle Y, U \rangle \langle Y, Z \rangle \langle W, T \rangle + \langle Y, U \rangle \langle Y, T \rangle \langle Z, W \rangle, \]
\[ I_3 := \langle U, W \rangle \langle Y, Z \rangle \langle Y, T \rangle + \langle U, Z \rangle \langle Y, W \rangle \langle Y, T \rangle + \langle U, T \rangle \langle Y, Z \rangle \langle Y, W \rangle, \]
\[ I_4 := \langle Y, U \rangle \langle Y, W \rangle \langle Y, Z \rangle \langle Y, T \rangle. \]
Then $\Sigma'_1$ and $\Sigma'_2$ can be re-written as

$$\Sigma'_1 = g_y I_1 + (1 - g_y) \frac{I_2}{\|Y\|_2},$$

$$\Sigma'_2 = g_y I_3 + 3(1 - g_y) \frac{I_4}{\|Y\|_2}. \tag{2.8}$$

It now follows from (2.6), (2.7) and (2.8) that

$$\nabla^4 h_y(U, W, Z, T) = I_1 \frac{g_y^2}{\|Y\|^2} + \frac{I_2}{\|Y\|^2} \left( \frac{3g_y^3 - 3g_y^2}{\|Y\|^2} - 1 + 2g_y \right)$$

$$+ I_3 \left( \frac{3g_y^3 - 3g_y^2}{\|Y\|^2} + g_y \right)$$

$$+ I_4 \left( \frac{15g_y^2 - 15g_y^3}{\|Y\|^2} + 4 - 9g_y \right)$$

$$- \langle Z, T \rangle \langle U, W \rangle g_y + \langle Z, T \rangle \langle Y, W \rangle \langle Y, U \rangle \frac{g_y}{\|Y\|^2} (g_y - 1). \tag{2.9}$$

We have finished computing up to order four derivative tensors of the squared distance function on spheres. These results will be used to derive conditions for the differentiability of the Fréchet function in in the next section.

### 3 Differentiability conditions of the Fréchet function

From now on, suppose that $Q$ which has a distribution function $f$ with respect to the volume measure on $S^d$, i.e.

$$dQ = fdV,$$

where $dV$ is the volume element of $S^d$. Fix a point $p \in S^d$, results from the previous part (c.f. (2.1), (2.3), (2.9) imply that the squared distance function $h_y$ has the fourth derivative everywhere except at the cut locus $\mathcal{C}_y$ of $y$.

It follows from the Leibniz integral rule that the Fréchet function function $F(x) = \int_{S^d} h_y(x) dQ(y)$ is differentiable of order $n$ if for every $x \notin \mathcal{C}_y$ the function $h_y$ is continuously differentiable up to order $n$ and the tensor $\nabla^n h_y(p)$ is integrable (in $y$) at $p$. In particular, for the Fréchet function to be differentiable of order 4 at $p$, it is suffices to find (sufficient) conditions for the convergence of the following integrals

$$\nabla F(T) = \int_{S^d} \nabla h_y(T) p dQ(y),$$

$$\nabla^2 F(Z, T) = \int_{S^d} \nabla^2 h_y(Z, T) p dQ(y), \tag{3.1}$$

$$\nabla^3 F(W, Z, T) = \int_{S^d} \nabla^3 h_y(W, Z, T) p dQ(y),$$

$$\nabla^4 F(U, W, Z, T) = \int_{S^d} \nabla^4 h_y(U, W, Z, T) p dQ(y),$$
where $U$, $W$, $Z$, $T$ are unit vector fields in $\mathcal{X}(S^d)$. Choose a polar parametrization on $S^d$ so that $p$ has coordinate $(0, 0, \ldots, 0)$. Let $\Omega := [0, \pi]^{d-1} \times [0, 2\pi]$ and define the following parametrization of $S^d$

$$
\begin{align*}
\varphi : \Omega &\to S^d \subset \mathbb{R}^{d+1} \\
\varphi &\equiv (\varphi_1, \ldots, \varphi_d) \mapsto (x_1, \ldots, x_{d+1}), \\
x_1 &= \cos \varphi_1, \\
x_2 &= \sin \varphi_1 \cos \varphi_2, \\
\ldots \\
x_{d+1} &= \sin \varphi_1 \sin \varphi_2 \ldots \sin \varphi_d,
\end{align*}
$$

(3.2)

where $\varphi_1, \ldots, \varphi_{d-1} \in [0, \pi]$, $\varphi_d \in [0, 2\pi]$. So $p$ has coordinate $(0, 0, \ldots, 0)$ and its antipode $C_p$ has coordinate $(\pi, 0, \ldots, 0)$. Suppose that a point $y$ has coordinate $(\varphi_1, \ldots, \varphi_d)$ then

$$
d_y(p) = ||Y(p)|| = \varphi_1,
$$

(3.3)

and

$$
g_y(p) = ||Y(p)|| \cot(||Y(p)||) = \varphi_1 \cot \varphi_1.
$$

(3.4)

Under the parametrization $\varphi$, the volume element of $S^d$ is

$$
dV = \sin^{d-1} \varphi_1 \ldots \sin \varphi_d d\varphi.
$$

Let $f_p$ be the pullback of $f$ under the parametrization $\varphi$ in (3.2), then

$$
dQ = f_p(\varphi) \sin^{d-1} \varphi_1 \ldots \sin \varphi_d d\varphi.
$$

It follows from (2.2), (2.5) and (2.9) that as $y$ approaches the antipode of $p$, $g_y^{j-1}(p)$ is the only unbounded term in the expression of $\nabla^j h_y(p) dQ(y)$. Hence, the integrability of $\nabla^j h_y(p) dQ(y)$ depends on the integrability of $g_y^{j-1}(p)$ for $j = 1, \ldots, 4$. It then suffices to require that the following integral converges.

$$
\int_{S^d} g_y^{j-1}(p) dQ(y) = \int_{\Omega} \varphi_1^{j-1} \cot^{j-1}(\varphi_1) f_p(\varphi) \sin^{d-1} \varphi_1 \ldots \sin \varphi_d d\varphi \\
= \int_{\Omega} \varphi_1^{j-1} \cos^{j-1}(\varphi_1) f_p(\varphi) \sin^{d-j} \varphi_1 \sin^{d-2} \varphi_2 \ldots \sin \varphi_d d\varphi
$$

(3.5)

for $j = 1, 2, \ldots, 4$. The following sufficient condition for the differentiability of the Fréchet function is a consequence of (3.5).

**Proposition 3.1** Given a measure $Q$ with distribution function $f$ on the $d$-dimensional sphere $S^d$. Fix a point $p \in S^d$, suppose that there exists an $\epsilon$-ball $B_{\epsilon}(C_p)$ centered at $C_p$ such that

i. $f$ is bounded on $B_{\epsilon}(C_p)$ when $d \geq j$, or

ii. $f$ vanishes on $B_{\epsilon}(C_p)$ when $d < j$. 

8
Then the Fréchet function $F(x) = \int_{S^d} d^2(x,y) dQ(y)$ is differentiable of order $j$, $j \leq 4$ in an open neighborhood of $p$.

Proof: Let $\Omega_\epsilon = \{ \varphi \in \Omega : \varphi_1 \in (\pi - \epsilon, \pi) \}$ be the preimage under the parametrization map $r$ of $B_\epsilon(C_p)$. Conditions (i) and (ii) translates into

1. $f_p$ is bounded on $\Omega_\epsilon$ when $d \geq j$, or,
2. $f_p$ vanishes on $\Omega_\epsilon$ when $d < j$.

First, we assume that $d \geq j$ and $f_p$ is bounded on $\Omega_\epsilon$. Write the integral in (3.5) as

$$
\int_{\Omega_\epsilon} \varphi_1^{j-1} \cos^{j-1}(\varphi_1) f_p(\varphi) \sin^{d-j}(\varphi_1) \sin^{d-2} \varphi_2 \ldots \sin \varphi_d d\varphi 
= \int_{\Omega_\epsilon} \varphi_1^{j-1} \cos^{j-1}(\varphi_1) f_p(\varphi) \sin^{d-j}(\varphi_1) \sin^{d-2} \varphi_2 \ldots \sin \varphi_d d\varphi 
+ \int_{\Omega_\epsilon} \frac{\varphi_1^{j-1}}{\sin^{j-1}(\varphi_1)} \cos^{j-1}(\varphi_1) f_p(\varphi) \sin^{d-j} \varphi_1 \sin^{d-2} \varphi_2 \ldots \sin \varphi_d d\varphi 
= I_1 + I_2.
$$

The integral $I_2$ converges as $\frac{\varphi_1^{j-1}}{\sin^{j-1}(\varphi_1)} \cos^{j-1}(\varphi_1)$ is bounded on $\Omega_\epsilon^C$. For the convergence of $I_1$, note that $f_p$ is bounded on $\Omega_\epsilon$ and so is the function under the integral of $I_1$. Thus, the integral (3.5) converges.

Now suppose that condition (2) holds, that means $d < j$ and $f_p(\varphi) = 0$, $\forall \varphi \in \Omega_\epsilon$. Then the integral (3.5) reduces to just $I_2$ and hence converges.

We have proved that the Fréchet function $F$ is differentiable of order $j$ at $p$. Next, observe that conditions (i) and (ii) still hold is we replace $p$ by any point $q \in B_\epsilon(p)$. Our arguments above then can be applied for $q$, so $F$ is differentiable of order $j$ at $q$. Thus $F$ is differentiable of order $j$ on $B_\epsilon(p)$. QED

4 Behavior of local Fréchet means on spheres

From now on, we assume that $Q$ is rotationally symmetric about $p$. Under the assumption of Proposition (3.1), the derivative tensors (up to order 4) of the Fréchet function are computed explicitly (c.f. (4.1), (4.2), (4.3). Let $f_p(\varphi)$ be the pullback distribution function of $f$ under the parametrization $r$ in (3.2). Then $f_p$ is a function on $\varphi_1$ only.

Since $Q$ is rotationally symmetric about $p$, so is the Fréchet function $F(x)$. Combining with the assumption that $F(x)$ is differentiable in a neighborhood of $p$, it suffices to study the behavior of $F(x)$ along a direction starting from $p$.

The first order tensor vanishes due to symmetry. We proceed to compute higher order tensors. Recall from the last section that $Y$ is the vector field $\nabla h_p$. Given a vector field $Z$, let $\theta(x) := \angle(Y(x), Z(x))$ be the angle between $Y$ and $Z$. It follows from (2.2), (2.3) and (2.9) that
\[ \nabla^2 h_y(Z, Z) = \|Z\|^2 (g_y \sin^2 \theta + \cos^2 \theta), \]
\[ \nabla^3 h_y(Z, Z, Z) = \frac{\|Z\|^3}{\|Y\|^2} (3g_y - 3g_y^2 - \|Y\|^2)(\cos \theta - \cos^3 \theta), \]
\[ \nabla^4 h_y(Z, Z, Z, Z) = \frac{\|Z\|^4}{\|Y\|^2} \left( 3g_y^2 - 3g_y^3 - \|Y\|^2 g_y \right) \]
\[ + \cos^2 \theta \left( 18g_y^3 - 18g_y^2 + 10\|Y\|^2 g_y - 4\|Y\|^2 \right) \]
\[ + \cos^4 \theta \left( 15g_y^2 - 15g_y - 9\|Y\|^2 g_y + 4\|Y\|^2 \right) \]
\[ = \frac{\|Z\|^4}{\|Y\|^2} \left( - \sin^2 \theta \left( 12g_y^2 - 12g_y^3 - 8\|Y\|^2 g_y + 4\|Y\|^2 \right) \right) \]
\[ + \sin^4 \theta \left( 15g_y^2 - 15g_y^3 - 9\|Y\|^2 g_y + 4\|Y\|^2 \right). \]

Assume, without loss of generality, that \( \theta = \varphi_2 \) and \( \|Z(p)\| = 1 \). Recall from (3.3) and (3.4) that
\[ \|Y(p)\| = \varphi_1, \]
\[ g_y(p) = \varphi_1 \cot \varphi_1. \]

Thus the second tensor of \( F(x) \) is rewritten as follows.
\[ \nabla^2 F(Z, Z)_p = \int_{\Omega} \left( \varphi_1 \cot \varphi_1 \sin^2 \varphi_2 + \cos^2 \varphi_2 \right) f_p(\varphi_1) \sin^{d-1} \varphi_1 \ldots \sin \varphi_n d\varphi \]
\[ = V(S^{d-2}) \int_0^\pi \int_0^\pi \left( \varphi_1 \cot \varphi_1 \sin^d \varphi_2 \right. \]
\[ \left. + \cos^2 \varphi_2 \sin^{d-2} \varphi_2 \right) \sin^{d-1} \varphi_1 f_p(\varphi_1) d\varphi_1 d\varphi_2, \]
where \( V(S^k) \) is the volume of the \( k \)-dimensional unit sphere. Set \( a_n = \int_0^\pi \sin^n x dx \) and use the following identity
\[ \sin^n x - \frac{n-1}{n} \sin^{n-2} x = - \frac{d}{dx} \left( \frac{1}{n} \cos x \sin^{n-2} x \right), \]
we have that
\[ a_n = \frac{n-1}{n} a_{n-2}. \]
Write $\nabla^2 F(Z, Z)_p$ as

$$\nabla^2 F(Z, Z)_p = V(S^{d-2}) \int_0^\pi \left( a_d \phi_1 \cot \phi_1 + a_{d-2} - a_d \right) \sin^{d-1} \phi_1 f(\phi_1) d\phi_1$$

$$= V(S^{d-2}) \int_0^\pi \frac{a_d}{d-1} \left( (d-1) \phi_1 \cos \phi_1 \sin^{d-2} \phi_1 + \sin^{d-1} \phi_1 \right) f(\phi_1) d\phi_1$$

$$= \frac{V(S^{d-2}) a_{d-2}}{d} \int_0^\pi f(\phi_1) d(\phi_1 \sin^{d-1} \phi_1)$$

The identity $V(S^d) = a_{n-1} V(S^{d-1})$ yields

$$\nabla^2 F(Z, Z)_p = \frac{V(S^{d-1})}{d} \int_0^\pi f(\phi_1) d(\phi_1 \sin^{d-1} \phi_1).$$

(4.1)

It is not hard to verify that the third order tensor vanishes due to symmetry.

$$\nabla^3 F(Z, Z, Z)_p = V(S^{d-2}) \int_0^\pi \int_0^\phi G(\phi_1) \cos \phi_2 \sin^d \phi_2 d\phi_2 d\phi_1$$

$$= 0,$$

with $G(\phi_1)$ is some function in $\phi_1$.

With a little more computation we get the result for the fourth order tensor.

$$\nabla^4 F(Z, Z, Z, Z)_p = \frac{a_d V(S^{d-2})}{d+2} \int_0^\pi \left( \sin \phi \cos \phi - \phi \cos^3 \phi \right) (3d - 9)$$

$$+ \phi \cos \phi \sin^2 \phi (7 - d) - 4 \sin^3 \phi \right) \sin^{d-4} \phi f(\phi) d\phi.$$ 

(4.3)

Since for $d = 2, 3$ and $\phi \in [0, \pi]$

$$\left( \sin \phi \cos \phi - \phi \cos^3 \phi \right) (3d - 9) + \phi \cos \phi \sin^2 \phi (7 - d) - 4 \sin^3 \phi < 0.$$ 

Therefore for $d < 4$, 

$$\nabla^4 F(Z, Z, Z, Z)_p < 0.$$ 

(4.4)

For $d \geq 4$ the tensor (4.3) becomes

$$\nabla^4 F(Z, Z, Z, Z)_p = \frac{a_d V(S^{d-2})}{d+2} \int_0^\pi f(\phi) d \left( \sin^{d-3} \phi (2\phi \sin^2 \phi + 3 \cos \phi \sin \phi - 3\phi) \right)$$ 

(4.5)

The first consequent of the above computations is a practical sufficient condition for $p$ to be a local Fréchet mean of $F(x)$. We have the following theorem.

**Proposition 4.1** Suppose that the measure $Q$ is rotationally symmetric about $p$ with distribution function $f$. Set

$$\alpha_d := \nabla^2 F(Z, Z)_p = \frac{V(S^{d-1})}{d} \int_0^\pi f(\phi) d(\phi \sin^{d-1} \phi),$$

we have the following claims.

11
1. If \( f \) is bounded on \( B_\epsilon(C_p) \) for some \( \epsilon > 0 \) and \( \alpha_d > 0 \) then \( p \) is a local minimum of the Fréchet function.

2. If \( d < 4 \), \( f \) vanishes on \( B_\epsilon(C_p) \) for some \( \epsilon > 0 \) and \( \alpha_d = 0 \) then \( p \) is a local maximum of the Fréchet function.

**Proof:** First note that the rotationally symmetric of \( Q \) implies that \( \nabla F_p = 0 \) and hence \( p \) is a critical point of \( F \).

Suppose that the conditions in claim 1 hold. The boundedness of \( f \) on \( B_\epsilon(C_p) \) ensures that the Fréchet function has derivative up to order 2, c.f. Proposition (3.1). It then follows from (4.1) that \( \alpha_d > 0 \) implies \( \nabla^2 F(Z, Z)_p > 0 \), \( \forall Z \in \mathcal{X}(S^d) \). Thus, \( p \) is a local minimum of \( F \).

Suppose that the condition in the second claim hold. Proposition (3.1) tells us that the Fréchet function has derivative up to order 4. It now follows from (4.2), (4.3) and \( \alpha_d = 0 \) that the function \( F \) when restricted to the geodesic tangent to \( Z(p) \) has a local maximum at \( p \). Since \( Z \) can be chosen freely and \( F \) is rotationally symmetric, \( p \) is a local maximum of \( F \).

**QED**

**Corollary 4.2**

i. The first result of proposition 4.1 confirmed a result in [Le98] that when \( f(\varphi) \) is nondecreasing and strictly decreasing in a measurable set then \( p \) is a local Fréchet mean.

ii. The second result of proposition 4.1 implies that smeary effect cannot occur in spheres of dimensions 2 and 3 with probability distributions that are rotationally symmetric about the mean and give zero measure to an open neighborhood of the mean’s cut locus. This result will be discussed in Section 5.

### 5 Central Limit Theorems

Two versions of the Central Limit Theorem are given. The first one (Theorem 5.1) is a spherical version of classical CLT on manifolds shown in [BL17] with an explicit limit distribution and more practical assumptions. The second is the smeary case (Definition 5.2) which was studied in [EHIS]. In this study, we show that smeary CLT does not occur for absolutely distribution in dimension 2 and 3 (Corollary 5.3). In dimension greater than 4, a sufficient condition for a 2-smeary CLT in high dimension \( d \geq 4 \) is given (Theorem 5.2).

Throughout the section, assume that: (1) the measure \( Q \) has a unique Fréchet mean \( p \); (2) \( Q \) is rotationally symmetric about \( p \); and (3) its distribution function is bounded in an open neighborhood of \( C_p \) when \( d \geq 4 \) or \( Q \) vanishes in an open neighborhood of \( C_p \) when \( d = 2, 3 \).
5.1 The classic case

Suppose that two vector fields $Z, T \in \mathcal{X}(S^d)$ are orthonormal at $p$. Then (2.2) gives

$$\nabla^2 h_y(Z, T) = -\frac{\langle Y, Z \rangle}{\|Y\|^2}(y - 1),$$

and hence

$$\nabla^2 F(Z, T)_p = -\int_{S^d} \frac{\langle \exp_p^{-1}(y), Z \rangle_p \langle \exp_p^{-1}(y), T \rangle_p}{\langle \exp_p^{-1}(y), T \rangle_p} (g_y(p) - 1) dQ(y). \tag{5.1}$$

Let $A$ be a reflection on $T_p S^d$ that fixes $Z(p)$ and send $T(p)$ to $-T(p)$. Since $Q$ is rotationally symmetric about $p$, it is fixed under the exponent of $A$,

$$\tilde{A} := \exp_p(A) : S^d \to S^d$$

$$y \mapsto \exp_p(A \exp_p^{-1}(y)).$$

In other words, $dQ(y) = dQ(\tilde{A}(y))$. For the sake of simplicity, we will write $\tilde{A}y$ for $\tilde{A}(y)$. Since $d(y, p) = d(\tilde{A}y, p)$, we have

$$\nabla^2 F(Z, T)_p = -\int_{S^d} \frac{\langle \exp_p^{-1}(\tilde{A}y), Z \rangle_p \langle \exp_p^{-1}(\tilde{A}y), T \rangle_p}{\langle \exp_p^{-1}(\tilde{A}y), T \rangle_p} (g_y(p) - 1) dQ(y)$$

$$= -\int_{S^d} \frac{\langle A \exp_p^{-1}(y), Z \rangle_p \langle A \exp_p^{-1}(y), T \rangle_p}{\langle A \exp_p^{-1}(y), T \rangle_p} (g_y(p) - 1) dQ(y)$$

$$= -\int_{S^d} \frac{\langle \exp_p^{-1}(y), AZ \rangle_p \langle \exp_p^{-1}(y), AT \rangle_p}{\langle AZ \rangle_p} (g_y(p) - 1) dQ(y)$$

$$= -\int_{S^d} \frac{\langle \exp_p^{-1}(y), Z \rangle_p \langle \exp_p^{-1}(y), T \rangle_p}{\langle AZ \rangle_p} (g_y(p) - 1) dQ(y)$$

$$= -\nabla^2 F(Z, T)_p.$$

Thus $\nabla^2 F(Z, T)_p = 0$. Combining this identity with (4.1) we obtain

$$\nabla^2 F(Z, T)_p = \alpha_d \mathbb{I}, \tag{5.2}$$

where $\alpha_d = \frac{V(S^{d-1})}{d} \int_0^\pi f(\varphi) d(\varphi \sin^{d-1} \varphi)$ as mentioned in proposition 4.1 and $I$ is the identity map. Therefore, when $\alpha_d > 0$ the Hessian of the Fréchet function at $p$ is positive definite and it is $\alpha_d \mathbb{I}$. Apply this result to Theorem 11 in [EH18] we obtain the following CLT.

**Theorem 5.1** Suppose $Q$ is a rotationally symmetric measure about a point $p$ on $S^d$, $d \geq 2$, with density function $f(\varphi)$ where $\varphi$ is the distance from $p$. Let $X_n$ be i.i.d. $S^d$-valued random variables with common distribution $Q$ and $Q_n = \frac{1}{n} \sum_1^n \delta_{X_i}$, the empirical distribution.

Suppose that
i. the function $f$ is bounded on an open neighborhood of $C_p$;

ii. $p$ is the unique Fréchet mean of the Fréchet function; and

iii. $\alpha_d > 0$.

Let $p_n$ be a measurable choice of the Fréchet mean (set) of the empirical distribution $Q_n$ and $Z_n := \exp_{p_n}^{-1} p$ be the inverse of $p_n$ under the exponential map from the tangent space $T_p S^n$ of $S^n$ at $p$. Also let $\Lambda$ be the covariant metric of the pushforward of $Q$ on $T_p S^d$ under $\exp_p^{-1}$. Then

$$n^{1/2} Z_n \xrightarrow{D} \mathcal{N}(0, \alpha_d^{-2} \Lambda).$$

Proof: It suffices to check the assumption 6 in [EH18] about the smoothness of the Fréchet function. It is clear from (5.2) and the symmetry of $F$ that for $q$ close to $p$

$$F(q) = F(p) + \alpha_d d^2(p, q) + o(d^2(p, q)),$$

which is the assumption 6 in [EH18] for $r = 2$. QED

5.2 The smeary case

We first recall the definition of smeary CLT in [EH18].

**Definition 5.2** Given a probability space $(\Omega, \mathcal{B}, P)$ and a number $k > 0$. A sequence of random vectors $X_n : \Omega_n \rightarrow \mathbb{R}^m$ with $\Omega_n \in \mathcal{B}, P(\Omega_n) \rightarrow 1$ as $n \rightarrow \infty$ is $k$-smeary with limit distribution of $X : \Omega \rightarrow \mathbb{R}^m$ if

$$n^{1/k+1} X_n \xrightarrow{D} X.$$

Suppose that $f$ satisfies assumptions in Proposition 3.1 with $d = 2, 3$ and $j = 4$. Proposition 4.1 gives the following consequence.

**Corollary 5.3** In low dimension, $d = 2, 3$, suppose that

i. $Q$ has a unique Fréchet mean $p$;

ii. $Q$ is absolutely continuous and rotationally symmetric about its mean $p$; and

iii. $Q$ gives zero mass to an open neighborhood of the cut locus of $p$.

Then there is no smeary effect on the unit sphere $S^d$.

Proof: Under the given conditions, proposition 4.1 implies that the Hessian of the Fréchet function at $p$ has to be positive. Thus, the CLT behaves classically. QED

In high dimension ($d \geq 4$), however, smeary effect does occur and it does more likely as the dimension increases.

Recall from (4.2) and (4.5) that

$$\nabla^3 F(Z_n, Z_n, Z_n) = 0,$$

$$\nabla^4 F(Z_n, Z_n, Z_n, Z_n) = \|Z\|^4 \beta_n,$$

(5.3)
with
\[ \beta_d := \frac{a_d V(S^{d-2})}{d+2} \int_0^\pi f(\varphi)d\left(\sin^{n-3}\varphi(2\varphi\sin^2\varphi + 3\cos\varphi\sin\varphi - 3\varphi)\right). \]

Taylor expansion of \( F \) at \( p \) along \( Z_n \) gives
\[
F(p_n) = F(p) + \nabla F(Z_n) + \frac{1}{2} \nabla^2 F(Z_n, Z_n) + \frac{1}{6} \nabla^3 F(Z_n, Z_n, Z_n) \\
+ \frac{1}{24} \nabla^4 F(Z_n, Z_n, Z_n, Z_n) + o(\|Z_n\|^4).
\]

For the moment we assume that \( \nabla^2 F(Z_n, Z_n) = 0 \) and \( \nabla^4 F(Z_n, Z_n, Z_n, Z_n) > 0 \), i.e. \( \alpha_n = 0 \) and \( \beta_n > 0 \). The expansion is simplified to
\[
F(p_n) = F(p) + \frac{1}{24} \|Z_n\|^4 \beta_n + o(\|Z_n\|^4). \tag{5.4}
\]

This is power expansion of order 4 of the Fréchet function at \( p \). Apply this result to Theorem 11, \[EH18\] we get a 2-smeary CLT for \( Z_n \).

**Theorem 5.4** Suppose that the measure \( Q \) on \( S^d \), \( d \geq 4 \) is absolutely continuous and rotationally symmetric about its mean \( p \) with distribution function \( f(\varphi(q)) \) where \( \varphi(q) \) is the distance from \( p \) to \( q \). In addition, suppose that \( Q \) satisfies the following conditions.

i. \( Q \) has a unique Fréchet mean \( p \);

ii. \( f \) is bounded in an open neighborhood of the cut locus \( C_p \);

iii. \( \alpha_d = \frac{V(S^{d-1})}{d} \int_0^\pi F(\varphi)d(\varphi\sin^{d-1}\varphi) = 0 \); and

iv. \( \beta_d = \frac{V(S^{d-2})}{d+2} \int_0^\pi \sin^d xdx \int_0^\pi f(\varphi)d\left(\sin^{n-3}\varphi(2\varphi\sin^2\varphi + 3\cos\varphi\sin\varphi - 3\varphi)\right) > 0 \)

Let \( Z_n = (z_{n,1}, \ldots, z_{n,m}) \) then
\[
n^{1/2} (|z_{n,1}|^2, \ldots, |z_{n,d}|^2) \xrightarrow{D} N(0, \frac{3}{2} \beta_d^{-2} \Lambda).
\]

**Proof:** The proof follows directly from (5.4) and Theorem 11, \[EH18\]. QED

**Remark 5.5** Since we can get the radius \( R \) sphere from multiplying the riemannian metric of the unit sphere with \( R^2 \), the signs of the derivative tensors of \( F \) remain unchanged if we replace the unit sphere in Theorem 5.4 by a sphere of radius \( R \). Thus, for spheres of arbitrary radius \( R \), conditions for smeary CLT in Theorem 5.4 remain the same. Therefore, at least for the case of constant sectional curvature, we showed here that the occurrence of the smeary effect depends largely on the dimension of a manifold as long as its sectional curvature is positive.

Conditions \( \alpha_d = 0 \) and \( \beta_d > 0 \) are not hard to archive, especially in high dimensions. Below we give an example of a piecewise constant function \( f \) such that conditions (ii), (iii), and (iv) hold. However, the example we introduce here only give a CLT for local Fréchet mean at \( p \) since we are unable to verify the uniqueness of the mean. Examples for global Fréchet mean with rotationally symmetric distribution and a singular mass at the mean is presented in [Elt19].
**Example 5.6** We need the following conditions on $f(\varphi)$.

\[
\int_{0}^{\pi} f(\varphi)d(\varphi \sin^{d-1} \varphi) = 0, \\
\int_{0}^{\pi} f(\varphi)d\left(\sin^{n-3} \varphi(2\varphi \sin^2 \varphi + 3 \cos \varphi \sin \varphi - 3\varphi)\right) > 0.
\]

Which is equivalent to

\[
\int_{0}^{\pi} f(\varphi)d(\varphi \sin^{d-1} \varphi) = 0 \\
\int_{0}^{\pi} f(\varphi)d\left(\sin^{d-3} \varphi \cos \varphi(\sin \varphi - \varphi \cos \varphi)\right) > 0. 
\]

(5.5)

Set $g_1(\varphi) := \varphi \sin^{d-1} \varphi$ and $g_2(\varphi) := \sin^{d-3} \varphi \cos \varphi(\sin \varphi - \varphi \cos \varphi)$. Note that $g_2$ is positive on $(0, \pi/2)$. The graphs of $g_2$ with $d = 10$ are depicted below.

![Graph of the function $g_2$ with $d = 10$ and examples of $\phi_1$ and $\phi_2$.](image)

Figure 1: Graph of the function $g_2$ with $d = 10$ and examples of $\phi_1$ and $\phi_2$.

Let $\phi_1 \in (0, \pi/2)$ and $\phi_2 = \pi - \epsilon$ with some small $\epsilon$. Suppose that $f(\varphi)$ is given by the following formula

\[
f(\varphi) = \begin{cases} 
  c_1 & \text{if } \varphi \in [0, \phi_1], \\
  c_2 & \text{if } \varphi \in [\pi/2, \phi_2], \\
  0 & \text{otherwise.}
\end{cases}
\]

Then (5.5) is equivalent to

\[
c_1 g_1(\phi_1) + c_2 g_1(\phi_2) - c_2 \frac{\pi}{2} = 0, \\
g_2(\phi_1) + g_2(\phi_2) > 0.
\]

(5.6)
The second condition can be easily obtained by choosing $\epsilon$ sufficiently small. In particular, choose $\epsilon$ such that
\[
\left( \frac{\sin \phi_1}{\sin \epsilon} \right)^{d-3} = \frac{\pi}{\cos \phi_1 (\sin \phi_1 - \phi_1 \cos \phi_1)},
\]
or
\[
\epsilon = \arcsin \left( \frac{\sin \phi_1}{\sqrt{\cos \phi_1 (\sin \phi_1 - \phi_1 \cos \phi_1)}} \right). \tag{5.7}
\]
The first condition in (5.6) is equivalent to
\[
\frac{c_1}{c_1} = \frac{\pi - 2\epsilon \sin^{d-1} \epsilon}{2\phi_1 \sin^{d-1} \phi_1}. \tag{5.8}
\]

To illustrate, the measure $Q$ is uniformly distributed on a lower cup from the South pole to the longitude of $\phi_1$ with a constant distribution function $f_1 = c_1$ and is uniformly distributed on a upper strip from the equator to the longitude of $\pi - \epsilon$ with a constant distribution function $f_2 = c_2$.

**Remark 5.7** It follows from (5.7) that if we fix $\phi_1$ then $\epsilon \to \phi_1$ and so $\phi_2 \to \pi - \phi_1$ as $d \to \infty$. It means that in high dimension, smeary effect can happen with a uniformly distributed cup in the bottom and a uniformly distributed thin upper strip near the equator. For example, the case $\phi_1 = 0$ is studied in [Elt19]. In that paper, the author showed that $p$ is a global Fréchet mean for some $\phi_2$ and $\phi_2$ converges to $\pi/2$ as the dimension $d$ grows.
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