The Power Spherical distribution

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Abstract

There is a growing interest in probabilistic models defined in hyper-spherical spaces, be it to accommodate observed data or latent structure. The von Mises-Fisher (vMF) distribution, often regarded as the Normal distribution on the hyper-sphere, is a standard modeling choice: it is an exponential family and thus enjoys important statistical results, for example, known Kullback-Leibler (KL) divergence from other vMF distributions. Sampling from a vMF distribution, however, requires a rejection sampling procedure which besides being slow poses difficulties in the context of stochastic backpropagation via the reparameterization trick. Moreover, this procedure is numerically unstable for certain vMFs, e.g., those with high concentration and/or in high dimensions. We propose a novel distribution, the Power Spherical distribution, which retains some of the important aspects of the vMF (e.g., support on the hyper-sphere, symmetry about its mean direction parameter, known KL from other vMF distributions) while addressing its main drawbacks (i.e., scalability and numerical stability). We demonstrate the stability of Power Spherical distributions with a numerical experiment and further apply it to a variational auto-encoder trained on MNIST. Code at: github.com/nicola-decao/power_spherical

1. Introduction

Manifold learning and machine learning applications of directional statistics (Sra, 2018) have spurred interest in distributions defined in non-Euclidean spaces (e.g., simplex, hyper-torus, hyper-sphere). Examples include learning rotations (i.e., SO(n), Falorsi et al., 2018; 2019) and hierarchical structures on hyperbolic spaces (Mathieu et al., 2019; Nagano et al., 2019). Hyper-spherical distributions, in particular, find applications in clustering (Banerjee et al., 2005; Bijral et al., 2007), mixed-membership models (Reisinger et al., 2010), computer vision (Liu et al., 2017), and natural language processing (Kumar & Tsvetkov, 2019).

The von Mises-Fisher distribution (vMF; Mardia & Jupp, 2009) is a natural and standard choice for densities in hyper-spheres. It is a two-parameter exponential family, one parameter being a mean direction and the other a scalar concentration, and it is symmetric about the former. Because of that, it is often regarded as the Normal distribution on spheres. Amongst other useful properties, it has closed-form Kullback-Leibler (KL) divergence with other vMF densities including the uniform distribution, one of its special cases. Thanks to the tangent-normal decomposition, sampling from a vMF, no matter its dimensionality, requires only sampling from a univariate marginal distribution. Unfortunately, the inverse cumulative density function (cdf) of this marginal is not known analytically, which prevents straightforward generation of independent samples. Fortunately, a rejection sampling procedure is known (Ulrich, 1984), but unsurprisingly, rejection sampling is inefficient.

In deep learning, an appealing use of the vMF distribution is as a random generator in stochastic and differentiable computation graphs. For that, we need a reparameterization trick to enable unbiased and low variance estimates of gradients of samples with respect to the vMF parameters (Rezende et al., 2014; Kingma & Welling, 2014).
We start with an overview of the vMF distribution, also introduced in some earlier works (Naesseth et al., 2017). This plays against widespread use of vMFs. For example, Davidson et al. (2018) successfully used the vMF distribution to approximate the posterior distribution of a hyper-spherical variational auto-encoder (VAE: Kingma & Welling, 2014), but they had to omit the correction term, while substituting the vMF with our proposed distribution.

Theorem 1 (9.1.2 in Mardia & Jupp (2009)). To overcome all of the vMF drawbacks, we propose the Power Spherical distribution. We start from the tangent-normal decomposition of vectors in hyper-spheres and specifically design a univariate marginal distribution that admits an analytical inverse cdf. This marginal is used to derive a distribution on hyper-spheres of any dimension. The resulting distribution is not an exponential family and is defined via a power law. Crucially, it is numerically stable and dispenses with rejection sampling for independent sampling. We verify the stability of the Power Spherical distribution with a numerical experiment as well as reproducing some of the experiments of Davidson et al. (2018) while substituting the vMF with our proposed distribution.

Contributions. We propose a new distribution defined on any $d$-dimensional hyper-sphere which

- has closed form marginal cdf and inverse cdf, thus it does not require rejection sampling;
- is fully reparameterizable without a correction term;
- is numerically stable in high dimensions and/or high concentrations.

2. Method

We start with an overview of the vMF distribution, also introducing results that help formulate the Power Spherical distribution. We then define the Power Spherical and present some of its properties such as mean, mode, variance, and entropy as well as its Kullback-Leibler divergence from a vMF and from a uniform distribution.

2.1. Preliminaries

Let $S^{d-1} = \{x \in \mathbb{R}^d : \|x\|_2 = 1\}$ be the hyper-spherical set. A key idea in directional distribution theory is the tangent-normal decomposition.

Theorem 1 (9.1.2 in Mardia & Jupp (2009)). Any unit vector $x \in S^{d-1}$ can be decomposed as

$$x = \mu t + v(1 - t^2)^{\frac{1}{2}},$$

with $t \in [-1, 1]$ and $v \in S^{d-2}$ a tangent to $S^{d-1}$ at $\mu$.

Corollary 1 (9.3.1 in Mardia & Jupp (2009)). The intersection of $S^{d-1}$ with the plane through $\mu \mu$ and normal to $\mu$ is a $(d - 2)$-sphere of radius $\sqrt{1 - t^2}$. Moreover, $t$ has density

$$p_{T}(t; d) \propto (1 - t^2)^{\frac{d-3}{2}} \quad \text{with} \quad t \in [-1, 1].$$

Importantly, it follows from Theorem 1 and Corollary 1 that every distribution that depends on $x$ only through $t = \mu^\top x$ can be expressed in terms of a marginal distribution $p_T$ and a uniform distribution $p_V$ on the subspace $S^{d-1}$. Density evaluation as well as sampling just requires dealing with the marginal $p_T$ as $p_V$ has constant density and it is trivial to sample from. An example from this class is the von Mises-Fisher distribution.

Definition 1. Let’s define a unnormalized density as

$$p_X(x; \mu, \kappa) \propto \exp(\kappa \mu^\top x) \quad \text{with} \quad x \in S^{d-1},$$

with direction $\mu \in S^{d-1}$ and concentration $\kappa \in \mathbb{R}_{>0}$. When normalized, this is the von Mises-Fisher distribution.

Theorem 2 (9.3.12 in Mardia & Jupp (2009)). The marginal $p_T(t; d, \kappa)$ of a von Mises-Fisher distribution is

$$p_T(t; d, \kappa) = C_T(\kappa, d) \cdot e^{\kappa t} \left(1 - t^2\right)^{\frac{d-3}{2}},$$

with normalizer $C_T(\kappa, d) =$

$$\left(\frac{\kappa}{2}\right)^{\frac{d-1}{2}} \left\{ \Gamma\left(\frac{d-1}{2}\right) \Gamma\left(\frac{1}{2}\right) \right\} I_{d-1}(\kappa) \right\}^{-1},$$

where $I_\nu(z)$ is the modified Bessel function of the first kind.

Although evaluation of $p_T$ is tractable, the Bessel function (Weisstein, 2002) (see Appendix A) is slow to compute and unstable for large arguments. Besides, $p_T$ does not admit a known closed-form cdf (nor its inverse). Thus, rejection sampling is normally used to draw samples from it (Ulrich, 1984).

2.2. The Power Spherical distribution

As all the issues of the vMF distribution stem from a problematic marginal, we address them by defining a new distribution that shares some basic proprieties of a vMF but none of its drawbacks. Namely i) it is rotationally symmetric about $\mu$, ii) it can be expressed in terms of a marginal distribution $p_T$, and iii) this marginal has closed-form and stable cdf (and inverse cdf).

Definition 2. Let’s define an unnormalized density as

$$p_X(x; \mu, \kappa) \propto \left(1 + \mu^\top x\right)^\kappa \quad \text{with} \quad x \in S^{d-1},$$

with direction $\mu \in S^{d-1}$ and concentration $\kappa \in \mathbb{R}_{>0}$. When normalized this is the Power Spherical distribution.
The Power Spherical distribution

Algorithm 1 Power Spherical sampling

**Input:** dimension $p$, direction $\mu$, concentration $\kappa$

Sample $z \sim \text{Beta}(Z; (d-1)/2 + \kappa, (d-1)/2)$

Sample $v \sim \mathcal{U}(S^{d-2})$

$t \leftarrow 2z - 1$

$y \leftarrow \{t; (\sqrt{1 - t^2})v^T\}^T$ \{concatenation\}

$\hat{u} \leftarrow e_1 - \mu \{e_1 \text{ is the base vector } [1, 0, \ldots, 0]^T\}$

$u = \frac{\hat{u}}{||u||_2}$

$x \leftarrow (I_d - 2nu^T)y \{I_d \text{ is the identity matrix } d \times d\}$

**Return:** $x$

As we show in Theorem 12 (Appendix C.1), the marginal of the Power Spherical instead.

| Property | Value |
|----------|-------|
| $E[X]$   | $\mu(\alpha - \beta)/(\alpha + \beta)$ |
| var($X$) | $\frac{2\alpha}{(\alpha + \beta)^2}((\beta - \alpha)\mu\mu^T + (\alpha + \beta)I_d)$ |
| Mode     | $\mu$ (for $\kappa > 0$) |
| H($T$)   | $H(\text{Beta}(\alpha, \beta)) + \log 2$ |
| H($X$)   | $\log N_X(\kappa, d) - \kappa\{\log 2 + \psi(\alpha) - \psi(\alpha + \beta)\}$ |

Table 1 summarizes some basic properties of the Power Spherical distribution. See Appendix C.3 for derivations. In particular, note that having a closed-form differential entropy allows using the Power Spherical in applications such as variational inference (VI; Jordan et al., 1999) and mutual information minimization.

**Kullback-Leibler divergence** The KL divergence between a Power Spherical $P$ and a uniform $Q = \mathcal{U}(S^{d-1})$ is

$$D_{KL}[P||Q] = -H(P) + H(Q).$$

See Theorem 17 (Appendix C.5) for the full derivation. Being able to compute the KL divergence from a uniform distribution in closed-form is useful in the context of variational inference as $Q$ can be used as a prior. Another important result we present here is a closed-form KL divergence of a Power Spherical distribution $P$ with parameters $\mu_p, \kappa_p$ from a vMF $Q$ with parameters $\mu_q, \kappa_q$, which evaluates to

$$-H(P) + \log C_X(\kappa_q, d) - \kappa_q\mu_q\mu_p^T(\alpha - \beta)(\alpha + \beta)$$

with $C_X(\kappa_q, d)$ the vMF normalizer (see Theorem 16 in Appendix C.5). This is valuable when using the Power Spherical to approximate a vMF, as we can assess the quality of the approximation. For example, if one has a vMF prior, it is then straightforward to use a Power Spherical approximate posterior in VI. If a vMF is necessary for a particular application, we can train with Power Spherical (enabling fast sampling and stable optimization) and then return the vMF that is closest to it in terms of KL.

3. Experiments

In this section we aim to show that Power Spherical distributions are more stable than vMFs, they are also faster to sample from, and lead to comparable performance when used in the context of variational auto-encoders.

**Stability** We tested numerical stability of both distributions for dimensions $d \in \{a \cdot 10^6\}$ and concentrations $\kappa \in \{a \cdot 10^6\}$ for all $a \in \{1, \ldots, 9\}, b \in \{0, \ldots, 5\}$. For

This is equal to the method of Davidson et al. (2018) (Algorithms 1 and 3) for sampling from a vMF where we use the marginal of the Power Spherical instead.
The Power Spherical distribution

(a) Stability of the vMF distribution. Ours does not have numerical issues in these intervals. Figure 2. Comparing stability (a) and running time (b) of the von Mises-Fisher and the Power Spherical distribution.

(b) Sampling time (on GPU) with $d = 64$ of a batch of 100 vectors of various concentrations. every combination of $(d, \kappa)$, we sample 10 vectors $x^{(i)}$ and compute the gradient $g^{(i)} = \nabla_{\kappa} \mu^T x^{(i)}$. If at least one of the samples $x^{(i)}$ or one of the gradients $g^{(i)}$ returns Not a Number (NaN), we mark $(d, \kappa)$ as unstable for that distribution. In Figure 2(a) we show the regions of instability. As intended, the Power Spherical does not present numerical issues in these intervals, while the vMF does. This makes our distribution more suitable where high dimensional vectors are needed such as for language modelling Kumar & Tsvetkov (2019).

**Efficiency** We also compare sampling efficiency between the Power Spherical and the vMF to highlight that rejection sampling is an undesirable bottleneck. We measured sampling time with $d = 64$ of a batch of 100 vectors of various concentrations $\kappa \in \{a \cdot 10^b \}$ with $a \in \{1, \ldots, 5\}$, $b \in \{0, \ldots, 4\}$. For every concentration $\kappa$ we computed mean and variance of 7 trials that consisted of computing the mean execution time (in milliseconds) sampling 100 times. Figure 2(b) shows the results. Sampling from a Power Spherical is at least $6 \times$ faster than sampling from a vMF. For some concentrations where the rejection ratio is worse, it is almost $20 \times$ faster. Noticeably, and differently from a vMF, sampling time is constant regardless of the concentration $\kappa$.

**Variational inference** Finally, we employed our Power Spherical distribution in the context of variational auto-encoders (Kingma & Welling, 2014). In particular, we replicated some of Davidson et al.’s (2018) experiments comparing the Power Spherical and the vMF on the MNIST dataset (LeCun et al., 1998). We implement a simple feed-forward encoder [784, 256, tanh, 128, tanh, $d$] and decoder [d, 128, tanh, 256, tanh 784] and optimize the evidence lower bound for 100 epochs for $d \in \{5, 10, 20, 40\}$. We used Adam (Kingma & Ba, 2014) with learning rate $10^{-3}$ and batch size 64. Table 2 shows importance sampling estimates (with 5k Monte Carlo samples) of log-likelihood and the evidence lower bound on the test set. We observe no substantial difference in performance between the two distributions. This shows, across dimensions, that the Power Spherical is sufficiently expressive to replace the vMF in this application. However, training with the Power Spherical was $>2 \times$ faster than with the vMF. One can notice that both log-likelihood and ELBO do not improve after $d = 40$. This is in line with Davidson et al.’s (2018) findings and a consequence of a shallow architecture. It is not the purpose of this experiment to show improvements on this task.

| Method | vMF | Power Spherical |
|--------|-----|----------------|
| $d = 5$ | $-114.51$ | $-114.49$ |
| $d = 10$ | $-97.37$ | $-97.46$ |
| $d = 20$ | $-93.80$ | $-93.70$ |
| $d = 40$ | $-98.64$ | $-98.63$ |

Table 2. Comparison between the vMF and Power Spherical distributions in a VAE on MNIST with different dimensional latent spaces $\mathbb{S}^{d-1}$. We show estimated (with 5k Monte Carlo samples) log-likelihood (LL) and evidence lower bound (ELBO) on test set.

4. Conclusion and future work

We presented a novel distribution on the $d$-dimensional sphere that, unlike the typically used von Mises-Fisher, $i)$ is numerically stable in high dimensions and concentration, $ii)$ has gradients of its samples with respect to its parameters, and $iii)$ does not require rejection sampling allowing faster computation and exact reparameterization gradient without a high variance correction term. We empirically show that our distribution is more numerically stable and faster to sample from compared to a vMF while preforming equally well in a variational auto-encoder setting. As shown in our experiments, high dimensional hyperspaces suffer from surface area collapse at the expense of the expressivity of latent space embeddings. Davidson et al. (2019) addressed some of these issues, future work might explore this direction further. Another future direction is to use the Power Spherical in combination with normalizing flows (Rezende & Mohamed, 2015). Though neural autoregressive flows (Huang et al., 2018; De Cao et al., 2019) have been shown to be remarkably flexible, they are still subject to topological constraints (Dinh et al., 2019; Cornish et al., 2019), which motivates extensions for complex manifolds (Brehmer & Cranmer, 2020; Wu et al., 2020) including spheres and tori (Rezende et al., 2020). In addition, a recent work by Falorsi & Forré (2020) extend Neural Ordinary Differential Equations (Chen et al., 2018) to arbitrary Riemannian manifolds allowing the use of continuous normalizing flow to such spaces.

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2On a NVIDIA Titan X 12GB GPU.
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A. Definitions

Definition 3. The Gamma function is:
\[ \Gamma(x) = \int_0^\infty u^{x-1} \exp(-u) \, du . \] (12)

Definition 4. The Beta function:
\[ B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)} . \] (13)

Definition 5. The incomplete Beta function is:
\[ B_x(a,b) = \int_0^x u^{a-1}(1-u)^{b-1} \, du . \] (14)

Definition 6. The regularized incomplete Beta function is:
\[ I_x(a,b) = \frac{B_x(a,b)}{B(a,b)} . \] (15)

Definition 7. The surface area of the hyper-sphere \( S^{d-1} \) is:
\[ A_{d-1} = \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} . \] (16)

Definition 8. The uniform distribution on \( S^{d-1} \) has constant density equal to the reciprocal of the surface area (Definition 7):
\[ p_X(x) = \frac{1}{A_{d-1}} . \] (17)

Definition 9. The modified Bessel function of the first kind is defined as
\[ I_v(z) = \left( \frac{1}{2} \right)^v \sum_{k=0}^\infty \frac{\left( \frac{1}{2} z^2 \right)^k}{k! \Gamma(v + k + 1)} . \] (18)

An useful integral function
\[ = \int (1 + x)^a (1 - x)^b \, dx \\
= 2^{a+b+1} B_{a+b+1} (a + 1, b + 1) + C . \] (19)

Definition 10. For a distribution \( P \) of a continuous random variable the differential entropy of the distribution \( X \) is defined as the integral
\[ H(P) = -\mathbb{E}_{p(x)} [ \log p(x) ] , \] (20)
where \( p \) denotes the probability density function of \( P \).

Definition 11. For distributions \( P \) and \( Q \) of a continuous random variable the Kullback-Leibler divergence is defined as the integral
\[ D_{KL}(P||Q) = -H(P) - \mathbb{E}_{p(x)} [ \log q(x) ] , \] (21)
where \( p \) and \( q \) denote the probability density function of \( P \) and \( Q \) respectively.

Definition 12. A random variable \( X \) is distributed according to the Beta distribution if its probability density function is
\[ B(\alpha, \beta)^{-1} x^{\alpha-1} (1 - x)^{\beta-1} , \] (22)
for \( x \in [0, 1] \) and zero elsewhere where \( \alpha \in \mathbb{R}^+ \) and \( \beta \in \mathbb{R}^+ \) are shape parameters.

B. Theorems

Theorem 3. The entropy of a random variable \( X \) Beta distributed is
\[ H(X) = \log B(\alpha, \beta) + (\alpha + \beta - 2) \psi(\alpha + \beta) - (\alpha - 1) \psi(\alpha) - (\beta - 1) \psi(\beta) , \] (23)
where \( \psi(x) = \frac{d}{dx} \log(\Gamma(x)) \).

Theorem 4. The expectation of \( X \) of a random variable \( X \) Beta distributed is
\[ \mathbb{E}[X] = \frac{\alpha}{\alpha + \beta} . \] (24)

Theorem 5. The expectation of \( \log X \) of a random variable \( X \) Beta distributed is
\[ \mathbb{E}[\log X] = \psi(\alpha) - \psi(\alpha + \beta) . \] (25)

Theorem 6. The expectation of \( X^2 \) of a random variable \( X \) Beta distributed is
\[ \mathbb{E}[X^2] = \frac{(\alpha + 1)\alpha}{(\alpha + \beta + 1)(\alpha + \beta)} . \] (26)

Theorem 7. The variance of \( X \) of a random variable \( X \) Beta distributed is
\[ \operatorname{var}[X] = \frac{\alpha \beta}{(\alpha + \beta)^2(\alpha + \beta + 1)} . \] (27)

Theorem 8. Given a bijective function \( f : \mathcal{X} \rightarrow \mathcal{Y} \) between two continuous random variables \( X \in \mathcal{X} \subseteq \mathbb{R}^d \) and \( Y \in \mathcal{Y} \subseteq \mathbb{R}^d \), a relation between the probability density functions \( p_Y(y) \) and \( p_X(x) \) is
\[ p_Y(y) = p_X(x) |\det J_{f(x)}|^{-1} , \] (28)
where \( y = f(x) \), and \(|\det J_{f(x)}|\) is the absolute value of the determinant of the Jacobian of \( f \) evaluated at \( x \).

Theorem 9. Given a bijective function \( f : \mathcal{X} \rightarrow \mathcal{Y} \) between two continuous random variables \( X \in \mathcal{X} \subseteq \mathbb{R}^d \) and \( Y \in \mathcal{Y} \subseteq \mathbb{R}^d \), a relation between the two respective entropies \( H(Y) \) and \( H(X) \) is
\[ H(Y) = H(X) + \int_X p_X(x) \log |\det J_{f(x)}| \, dx , \] (29)
where \( y = f(x) \), and \(|\det J_{f(x)}|\) is the absolute value of the determinant of the Jacobian of \( f \) evaluated at \( x \).
Theorem 10 (9.3.33 in Mardia & Jupp (2009)). Continuous distributions with rotational symmetry about a direction \( \mu \) and with probability density functions of the form \( p_X \propto g(\mu^\top x) \) have mean
\[
E[X] = E[T]\mu.
\]
(30)

Theorem 11 (9.3.34 in Mardia & Jupp (2009)). Continuous distributions with rotational symmetry about a direction \( \mu \) and with probability density functions of the form \( p_X \propto \) have variance
\[
\text{var}[X] = \text{var}[T]\mu^\top + \frac{1 - E[T^2]}{d-1} (I_d - \mu\mu^\top),
\]
(31)

where \( I_d \) is the \( d \times d \) identity matrix.

C. Derivations

C.1. The Power Spherical marginal

Theorem 12. Let \( S^{d-1} = \{ x \in \mathbb{R}^d : \|x\| = 1 \} \) be the hyper-spherical set. Let an unnormalized density be
\[
p_X(x; \mu, \kappa) \propto (1 + \mu^\top x)^\kappa \ 	ext{with} \ x \in S^{d-1},
\]
(32)

with \( x \in S^{d-1} \), direction \( \mu \in S^{d-1} \), and concentration parameter \( \kappa \in \mathbb{R}_{\geq 0} \). Let \( T \) bet a random variable that denotes the dot-product \( t = \mu^\top x \), then
\[
T = 2Z - 1 \ 	ext{with} \ Z \sim \text{Beta}(\alpha, \beta),
\]
(33)

where \( \alpha = \frac{d-1}{2} + \kappa \) and \( \beta = \frac{d-1}{2} \).

Proof. Given Corollary 1, the marginal distribution of the dot-product \( t \) is \( \propto (1 + t)^\kappa (1 - t^2)^{\frac{d-3}{2}} \) so its normalizer is
\[
N_T(\kappa, d) = \int_{-1}^{1} (1 + t)^\kappa (1 - t^2)^{\frac{d-3}{2}} \, dt
\]
(34)
\[
= \frac{2^{d+\kappa-2}}{B_1} \left( \frac{d-1}{2} + \kappa, \frac{d-1}{2} \right)
\]

\[
= 2^{d+\kappa-2} B \left( \frac{d-1}{2} + \kappa, \frac{d-1}{2} \right)
\]
(36)

It follows that the probability density function of the dot-product marginal distribution is \( p_T(t; \kappa, d) = \)
\[
N_T(\kappa, d)^{-1} (1 + t)^\kappa (1 - t^2)^{\frac{d-3}{2}}
\]
(38)
\[
= N_T(\kappa, d)^{-1} (1 + t)^{\frac{d-3}{2} + \kappa} (1 - t)^{\frac{d-3}{2}}
\]
(39)
\[
= N_T(\kappa, d)^{-1} (2z)^{\frac{d-3}{2} + \kappa - 1} (2 - 2z)^{\frac{d-3}{2} - 1}
\]
(40)
\[
= B(\alpha, \beta)^{-1} z^{\alpha-1} (1 - z)^{\beta-1}.
\]
(41)

where * indicates a substitution \( t = 2z - 1 \) and eventually \( \alpha = \frac{d-1}{2} + \kappa, \beta = \frac{d-1}{2} \). Notice that Equation 41 is a Beta distribution. Therefore, if we define the random variable \( Z \sim \text{Beta}(\alpha, \beta) \) turns out that \( T \) is simply \( T = 2Z - 1 \).

Corollary 2. Following Theorem 12, the marginal of a Power Spherical distribution has cumulative density function \( F(t; \kappa, d) = \)
\[
N_T(\kappa, d)^{-1} \int_{-1}^{t} (1 + x)^\kappa (1 - x^2)^{\frac{d-3}{2}} \, dx
\]
(42)
\[
= B(\alpha, \beta)^{-1} B_{\frac{d+\kappa-2}{2}} (\alpha, \beta)
\]
(43)
\[
= I_{\frac{d+\kappa-2}{2}} (\alpha, \beta)
\]
(44)

and inverse cumulative density function
\[
F^{-1}(y; \kappa, d) = 2I_{\frac{y}{\mu}}^{\frac{1}{2}} (\alpha, \beta) - 1.
\]
(45)

Corollary 3. Using Theorem 3 and 9 we derive the differential entropy of the marginal Power Spherical \( p_T \). Using \( t = 2z - 1 = f(z) \), \( \det J_{f(z)} = 2 \) for all \( z \), and then
\[
H(T) = H(Z) + \log 2
\]
(46)
\[
\overset{(23)}{=} \log B(\alpha, \beta) + (\alpha + \beta - 2)\psi(\alpha + \beta)
\]
\[
- (\alpha - 1)\psi(\alpha) - (\beta - 1)\psi(\beta) + \log 2.
\]
(47)

C.2. The normalized Power Spherical distribution

Theorem 13. The normalized density of the Power Spherical distribution is \( p_X(x; \mu, \kappa) = \)
\[
\left\{ 2^{\alpha + \beta} \pi^\beta \frac{\Gamma(\alpha)}{\Gamma(\alpha + \beta)} \right\}^{-1} (1 + \mu^\top x)^\kappa,
\]
(48)

with \( \alpha = \frac{d-1}{2} + \kappa \) and \( \beta = \frac{d-1}{2} \).

Proof. The Power Spherical is expressed via the tangent normal decomposition (Theorem 1) as a joint distribution between \( T \sim p_T(t; \kappa, d) \) (from Theorem 12) and \( V \sim U(S^{d-2}) \). Since \( T \perp V \), the Power Spherical normalized \( N_X(p, \kappa) \) is the product of the normalizer of \( p_T(t; \kappa, d) \) and the uniform distribution on \( S^{d-2} \) (whose probability is
constant on the $d - 2$-sphere – see Definition 8), that is
\[
N_X(\kappa, d) = N_T(\kappa, d) \cdot A_{d-2}
\]
\[
= 2^{\alpha + \beta} B(\alpha, \beta) \frac{2\pi^\beta}{\Gamma(\beta)}
\]
\[
= 2^{\alpha + \beta} \frac{\Gamma(\alpha)}{\Gamma(\alpha + \beta)}
\]
Thus, $p_X(x; \mu, \kappa) = N_X(\kappa, d)^{-1}(1 + \mu^\top x)^\kappa$.

C.3. Power Spherical properties

**Corollary 4.** Directly applying Theorem 10, the mean of a Power Spherical is
\[
E[X] = E[T] \mu = (2E[Z] - 1)\mu = \left(\frac{\alpha - \beta}{\alpha + \beta}\right) \mu,
\]
with $\alpha = \frac{d - 1}{2} + \kappa$, $\beta = \frac{d - 1}{2}$.

**Corollary 5.** Directly applying Theorem 11, the variance of a Power Spherical is $var[X] =$
\[
= \text{var}[T] \mu \mu^\top + \frac{1 - E[T^2]}{d - 1} (I_d - \mu \mu^\top)
\]
\[
= 4 \text{var}[Z] \mu \mu^\top + \frac{4 E[Z] - E[Z^2]}{2\beta} (I_d - \mu \mu^\top)
\]
\[
= 2 \text{var}[Z] \left(\frac{(\beta - \alpha) \mu \mu^\top + (\alpha + \beta) I_d}{(\alpha + \beta)^2 (\alpha + \beta + 1)}\right)
\]
with $\alpha = \frac{d - 1}{2} + \kappa$, $\beta = \frac{d - 1}{2}$ and $I_d$ is the $d \times d$ identity matrix.

**Theorem 14.** The mode of a Power Spherical with $\kappa > 0$ is
\[
\text{arg max}_{x \in S^{d-1}} p_X(x; \mu, \kappa) = \mu.
\]

**Proof.** We have $\text{arg max}_{x \in S^{d-1}} p_X(x; \mu, \kappa) =$
\[
= \text{arg max}_{x \in S^{d-1}} N_X(\kappa, d)^{-1}(1 + \mu^\top x)^\kappa
\]
\[
\kappa > 0 \rightarrow \text{arg max}_{x \in S^{d-1}} \log(1 + \mu^\top x)
\]
\[
= \text{arg max}_{x \in S^{d-1}} \mu^\top x = \mu.
\]

C.4. Power Spherical differential entropy

**Theorem 15.** The differential entropy of the Power Spherical $p_X$ that is $H(X) =$
\[
\log N_X(\kappa, d) - \kappa (\log 2 + \psi(\alpha) - \psi(\alpha + \beta))
\]
with $\alpha = \frac{d - 1}{2} + \kappa$, $\beta = \frac{d - 1}{2}$.

**Proof.** Applying Definition 10, $H(X) =$
\[
= -E[\log q(X)]
\]
\[
= \log N_X(\kappa, d) - \kappa \log(1 + \mu^\top X)
\]
\[
= \log N_X(\kappa, d) - \kappa (\log 2 + E_Z[\log Z])
\]
\[
= \log N_X(\kappa, d) - \kappa (\log 2 + \psi(\alpha) - \psi(\alpha + \beta)).
\]

C.5. Kullback-Leibler divergence with the von Mises-Fisher distribution

**Theorem 16.** The Kullback-Leibler divergence $D_{KL}(\text{Definition 11})$ between a Power Spherical distribution $P$ with parameters $\mu_p, \kappa_p$ and von Mises-Fisher and $Q$ with parameters $\mu_q, \kappa_q$ is $D_{KL}[P||Q] =$
\[
= -H(P) + \log C_X(\kappa_q, d) - \kappa_q \mu_q^\top \mu_p \left(\frac{\alpha - \beta}{\alpha + \beta}\right)
\]
with $\alpha = \frac{d - 1}{2} + \kappa$, $\beta = \frac{d - 1}{2}$.

**Proof.** Applying Definition 11, $D_{KL}[P||Q] =$
\[
= -H(P) - E_{p_X}[\log q(X)]
\]
\[
= -H(P) + \log C_X(\kappa_q, d) - \kappa_q \mu_q^\top E_{p_X}[T] \mu_p
\]
\[
= -H(P) + \log C_X(\kappa_q, d) - \kappa_q \mu_q^\top \mu_p \left(\frac{\alpha - \beta}{\alpha + \beta}\right).
\]
where $C_X(\kappa_q, d)$ is the von Mises-Fisher normalizer.

C.6. Kullback-Leibler divergence with $U(S^{d-1})$

**Theorem 17.** The Kullback-Leibler divergence $D_{KL}(\text{Definition 11})$ between a Power Spherical distribution $P$ and a uniform distribution on the sphere $Q = U(S^{d-1})$ is
\[
D_{KL}[P||Q] = -H(P) + H(Q)
\]

**Proof.** Applying Definition 11, $D_{KL}[P||Q] =$
\[
= -H(P) - E_{p_X}[\log q(X)]
\]
\[
= -H(P) + H(Q),
\]
where $H(Q) = \log A_{d-1}$ (from Definition 8).