Fast Python sampler for the von Mises Fisher distribution

Carlos Pinzón, Kangsoo Jung

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Carlos Pinzón
Inria, LIX

Kangsoo Jung
Inria, LIX

Abstract

This paper implements a method for sampling from the d-dimensional Von Mises Fisher distribution using NumPy, focusing on speed and readability. The complexity of the algorithm is $O(nd)$ for n samples, which is theoretically optimal taking into account that nd is the output size.

1 Introduction

The von Mises Fisher distribution (VMF), named after Richard von Mises [vM81] and Ronald Fisher [Fis53], is a probability distribution used in directional statistics and directional privacy mechanisms that generalizes the von Mises distribution (VM) for larger dimensions. The VM distribution has a circumference as domain, or equivalently the interval $[-\pi, \pi]$, while the domain of the d-dimensional VMF distribution is the $(d-1)$-sphere S^{d-1}, hence VM corresponds to VMF when $d = 2$.

For given parameters of mean direction $\mu \in S^{d-1}$ and concentration $\kappa \in (0, \infty)$, the density function of the VMF is given, for each point $x \in S^{d-1}$, by

$$p(x \mid \mu, \kappa) = C_d(\kappa) \exp(\kappa \mu \cdot x),$$

where the $\cdot$ denotes the dot product, i.e. the standard inner product in d-dimensions, and $C_d(\kappa)$ is a normalization constant that depends only on the dimensionality d and the concentration κ.

When $d = 2$, the domain is S^1, i.e. the circumference of radius 1 in $\mathbb{R}^2$, and letting θ_0 and θ be the angles that define μ and x respectively, the density function is given by $p(\theta \mid \theta_0, \kappa) = C_2(\kappa) \exp(\kappa \cos(\theta_0 - \theta))$, because $\mu \cdot x = |\mu|\,|x| \cos(\theta_0 - \theta) = \cos(\theta_0 - \theta)$. This formula coincides with that of the VM distribution in the form that it is typically presented, with its parameter varying in $[-\pi, \pi]$.

There exist implementations for VM in the main scientific Python packages SciPy [Sci23] and NumPy [Num23], but they do not implement the VMF in general (for $d \neq 2$). In this paper, we propose a fast implementation of the VMF that runs in $\Theta(n\,d)$, which is optimal, since $n \times d$ is also to the size of the output.

2 Related work

There are two Python implementations for sampling from the VMF distribution [ten23, Whi23]. Before introducing the main difference between our algorithm and these implementations, let us describe in detail the principles they follow.

◦ **Principle 1 (rotation).** Due to the rotational symmetry, it suffices to have a sampler that handles only $\mu = \hat{e}_d = (0, 0, ..., 0, 1)^\top$, because the resulting samples can be rotated afterwards towards the true μ. This rotation is carried out using a rotation matrix, which can be computed using Givens rotations and Householder reflections [Hou58].

◦ **Principle 2 (decomposition).** The sampling problem can be decomposed into computing the random angular deviation $\theta \in [0, \pi]$ between the output x and μ, and the random direction z in which the angle occurs.

Figure 2.1, taken from Weggenmann and Kerschbaum [WK21], depicts the decomposition principle for the case $d = 3$. The figure shows the angle θ between μ and x, and all the remaining orientation information, is captured in the $(d-1)$-dimensional unitary vector ξ. Since μ is fixed to be $\mu = \hat{e}_d = (0, 0, 1)$, we can embed $\xi = (\xi_1, \xi_2)$ in 3 dimensions as $z = (\xi_1, \xi_2, 0)$, so that it is perpendicular to μ. The problem of sampling from VMF can therefore be reduced to sampling θ and ξ separately, and letting the output (assuming $\mu = \hat{e}_d$) be $x = \cos(\theta)\mu + \sin(\theta)z$.

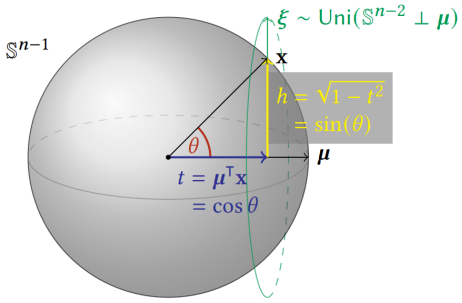

Figure 2.1: Decomposition into θ and ξ.

◦ **Principle 3 (Muller).** Sampling ξ can be done using the algorithm by Muller [Mul59]. More precisely, if $Y_1, ..., Y_{d-1} \sim \mathcal{N}(0, 1)$ are independent, and we let $Y = (Y_1, ..., Y_{d-1})^\top$, it is known that the unitary vector $\xi \coloneqq Y/|Y|$ is uniformly distributed on the $(d-2)$-sphere. For instance, when $d = 3$, ξ is a 2-dimensional vector taken from the 1-sphere (the circumference), and when $d = 2$, ξ is a 1-dimensional vector taken from the 0-sphere (the set $\{-1, 1\}$).

◦ **Principle 4 (Ulrich-Woods).** Sampling θ can be done using the algorithm by Ulrich [Ulr84], which was later revised and improved by Woods [Woo94]. It can be shown from the definition of the VMF distribution that the marginal distribution of the angle $\theta \in [0, \pi]$ is given for some constant $C'_d(\kappa)$ by

$$p(\theta \mid \mu, \kappa) = C'_d(\kappa)\,(\sin\theta)^{d-2} \exp(\kappa \cos\theta). \tag{2.1}$$

Ulrich and Woods propose a rejection method for generating samples θ that follow this distribution.

3 Algorithm

We propose to avoid the rotation step and to work entirely in the d-dimensional space. This means that the Muller method needs to be adjusted to produce vectors uniformly in $\{z \in S^{d-1} : z \perp \mu\}$ instead of $\{\xi \in S^{d-2}\}$. The Ulrich-Woods method, however, is left untouched, although it is vectorized to increase speed. The implementation is shown below.

```
import numpy as np

def random_VMF(mu, kappa, size=None):
    """
    Von Mises-Fisher distribution sampler with
    mean direction mu and concentration kappa.
    Source: https://hal.science/hal-04004568
    """
    # parse input parameters
    n = 1 if size is None else np.product(size)
    shape = () if size is None else tuple(np.ravel(size))
    mu = np.asarray(mu)
    mu = mu / np.linalg.norm(mu)
    (d,) = mu.shape
    # z component: radial samples perpendicular to mu
    z = np.random.normal(0, 1, (n, d))
    z /= np.linalg.norm(z, axis=1, keepdims=True)
    z = z - (z @ mu[:, None]) * mu[None, :]
    z /= np.linalg.norm(z, axis=1, keepdims=True)
    # sample angles (in cos and sin form)
    cos = _random_VMF_cos(d, kappa, n)
    sin = np.sqrt(1 - cos**2)
    # combine angles with the z component
    x = z * sin[:, None] + cos[:, None] * mu[None, :]
    return x.reshape((*shape, d))

def _random_VMF_cos(d: int, kappa: float, n: int):
    """
    Generate n iid samples t with density function given by
      p(t) = someConstant * (1-t**2)**((d-2)/2) * exp(kappa*t)
    """
    # b = Eq. 4 of https://doi.org/10.1080/03610919408813161
    b = (d - 1) / (2 * kappa + (4 * kappa**2 + (d - 1)**2)**0.5)
    x0 = (1 - b) / (1 + b)
    c = kappa * x0 + (d - 1) * np.log(1 - x0**2)
    found = 0
    out = []
    while found < n:
        m = min(n, int((n - found) * 1.5))
        z = np.random.beta((d - 1) / 2, (d - 1) / 2, size=m)
        t = (1 - (1 + b) * z) / (1 - (1 - b) * z)
        test = kappa * t + (d - 1) * np.log(1 - x0 * t) - c
        accept = test >= -np.random.exponential(size=m)
        out.append(t[accept])
        found += len(out[-1])
    return np.concatenate(out)[:n]
```

The function `random_VMF` takes as input parameters a vector μ of shape

`(d,)`, a floating point number κ, and an optional shape `size`, that follows the `numpy` ecosystem standards. More precisely, when `size` is not given, the function generates a single d-dimensional output vector; when it is an integer n, it generates n vectors and the output has shape (n, d); and when it is a shape tuple, say $(1, 100, 3)$, the output will have shape $(1, 100, 3, d)$.

The function `_random_VMF_cos` is used by `random_VMF`. This function generates angles θ that follow Equation (2.1) and returns their cosine. It uses the Ulrich-Woods [Woo94] method with vectorization to accelerate the process. The number of loops executed by this algorithm (hence also the complexity) is stochastic, but it typically is 2 and rarely exceeds 4. This occurs because, the acceptance rate of the Ulrich-Woods method is always above 65.9% (worst case), and is higher for large d or small κ. As a heuristic to increase speed, we take n samples on the first loop, out which a fraction is possibly rejected, and for the next iteration, if there are n' more samples needed, we take $n' + 50\%$. This extra overhead increases significantly the chances of the algorithm of needing only one extra round, at the expense of possibly computing more samples than needed. The increase of 50% is not done in the first round to account for the case when the acceptance rate is high (large d or small κ), in which most of the extra samples in the first round will be unused. In the worst case in which the first round rejects more than $100\% - 65.9\% = 34\%$, the next round will use a sample size of around $65.9\% \times 150\% \approx 100\%$ of n. We acknowledge that our empirically fast heuristic can be replaced with an even faster more refined heuristic that computes the optimal increase of samples, but probably at the cost of reducing simplicity and readability.

4 Experiments

We experimentally show that our implementation is faster while producing the same outputs as [ten23, Whi23], which are the existing sampling implementations from VMF distributions. Table 1 compares the execution time comparison of our implementation with the existing implementations [ten23, Whi23] when generating 1,000 samples. We compared the results while increasing the number of dimensions to 2, 3, 5, and 50 when kappa was 5 and 50, respectively. As can be seen from the results, the proposed implementation is more than 10 times faster than the existing implementations. The experimental environment is Intel Core i5-9400H CPU 2.50GHZ with 16GB ram and the OS is Windows.

Table 1: Execution time comparison

		d=2	d=3	d=5	d=50
κ=5	[Whi23]	10.28ms	9.01ms	8.54ms	7.75ms
	[ten23]	68.53ms	8.55ms	41.84ms	27.75ms
	[Our]	0.60ms	0.48ms	0.55ms	1.11ms
κ=50	[Whi23]	10.39ms	10.03ms	10.21ms	9.74ms
	[ten23]	60.76ms	8.85ms	52.30ms	50.96ms
	[Our]	0.61ms	0.58ms	0.65ms	1.29ms

Figures 4.1, 4.2, and 4.3 visualize samples generated from [Whi23] and the proposed implementation. It can be seen that the same distribution is created with the results when the dimension is 2, 3, and 4, respectively.

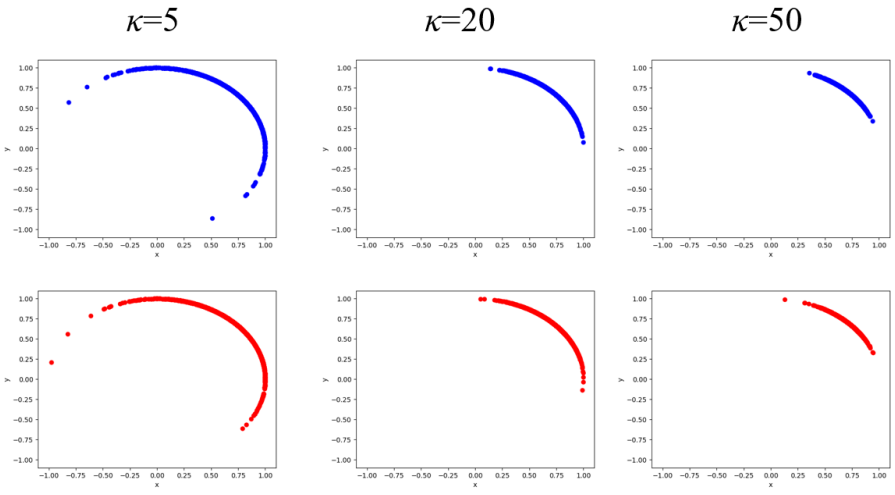

Figure 4.1: The figures in the first row are the outputs of sampling in 2-dimension from [Whi23] and the figures in the second row are the outputs of sampling in 2-dimension with our implementation.

5 Conclusion

Directional statistics are used in various fields such as animal navigation, tracking, image analysis, and applications in which the direction is more important than the magnitude, though, it has received less attention than statistics in Euclidean space. However, if the data are normalized to the unit norm and lie on the surface of S^{d-1}, directional statistics are more appropriate than Euclidean

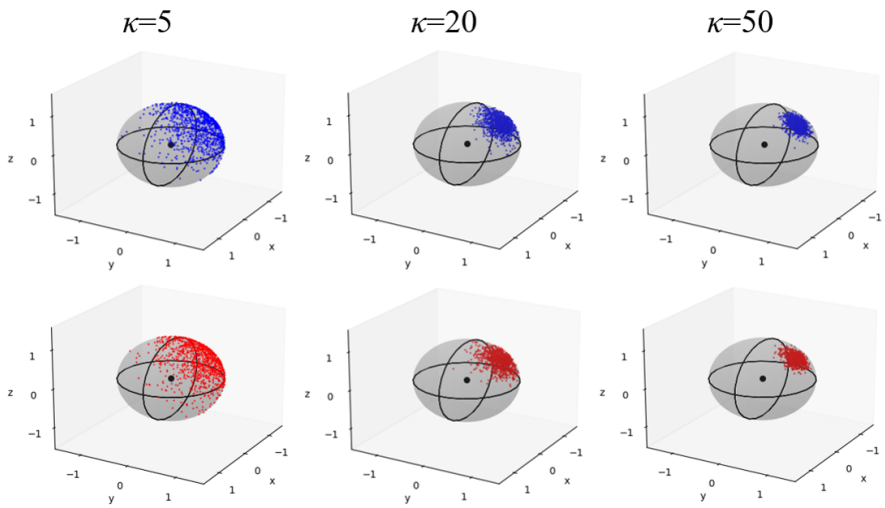

Figure 4.2: The figures in the first row are the outputs of sampling in 3-dimension from [Whi23] and the figures in the second row are the outputs of sampling in 3-dimension with our implementation.

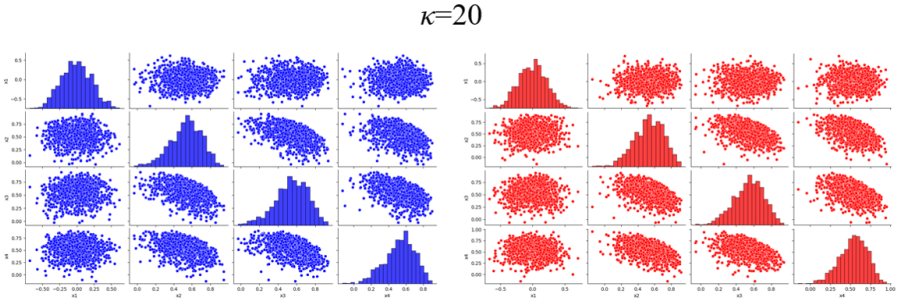

Figure 4.3: The left figures are the outputs of sampling in 4-dimension from [Whi23] and the right figures are the outputs of sampling in 4-dimension with our implementation.

statistics.

The von Mises Fisher distribution (VMF) has been used as a probability distribution in directional statistics, but its implementation is not being provided as python libraries. We intend to contribute to the field where directional statics are needed by proposing an implementation that produces the same outputs as existing implementations but is more than 10 times faster.

Acknowledgements

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