A Wrapped Trivariate Normal Distribution and Bayes Inference for 3-D Rotations

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Supplementary Material

This supplement consists of four sections. Section S1 provides a proof of Proposition 1 from the main manuscript, regarding the CLT for a triangular array of UARS rotations, and Section S2 establishes that the UARS class of rotations is closed under matrix compositions. Section S3 provides numerical evidence that family of the isotropic Matrix Fisher distributions is not closed under matrix compositions. Sections S1-S3 involve topics discussed in Section 2.2 of the main manuscript. Section S4 gives other conventions used to describe UARS densities.

S1 Justification of Proposition 1

Here we use distributional properties of UARS-rotations, along with verifying general CLT conditions for rotations established by Parthasarathy (1964) and re-iterated by Nikolayev & Savyolova (1997). Without loss of generality, suppose $\mathbf{S} = \mathbf{I}_3$. From the UARS construction (1), the expectation $E(\mathbf{O}_{i,n}) = a_n\mathbf{I}_3$ follows, where $a_n = \frac{1}{3} + \frac{2}{3}E[\cos(r_{i,n}/\sqrt{n})]$. By Taylor expansion, $E[\cos(r_{i,n}/\sqrt{n})] = 1 - \frac{\sigma^2}{2n} + e_n$, where $|e_n| \leq \pi^3/n^{3/2}$. It then holds that

$$\overline{\lim}_{n\to\infty} n\{1 - \det[E(\mathbf{O}_{i,n})]\} = \overline{\lim}_{n\to\infty} n\left[1 - \left(1 - \frac{\sigma^2}{3n} + e_n\right)^3\right]$$

is finite (equaling $\sigma^2 < \infty$) and that

$$\lim_{n\to\infty} n\left[\mathbf{I}_3 - E(\mathbf{O}_{i,n})\right] = \frac{\sigma^2}{3}\mathbf{I}_3.$$

By applying a result of Nikolayev & Savyolova (1997, Theorem 1), the proposition then follows where the concentration parameter in the isotropic Gaussian distribution on

$SO(3)$ (see Table 1) is determined by $\kappa_{IG} = \sqrt{3}/\sigma$ (i.e, determined by the limiting scaled difference between the identity matrix and the mean $E(\mathbf{O}_{i,n})$ of a UARS rotation used in the composition). $\square$

S2 Products of independent UARS-rotations

The following result shows that the UARS class of random rotations is closed under convolution.

Proposition 2 *Suppose $\mathbf{O}_1, \ldots, \mathbf{O}_n$ are independent (not necessarily identically distributed) random rotation matrices, each having some rotational distribution in the UARS class with mean rotation $\mathbf{I}_3$. Then, the rotational distribution of the product $\mathbf{O}_1 \cdots \mathbf{O}_n$ also belongs to the UARS class with mean rotation $\mathbf{I}_3$.*

To show the result, we use an alternative, but equivalent, definition of a UARS rotation. That is, if $|r|$ is randomly generated on $[0, \pi]$ and, conditional on $|r|$, $\mathbf{u}$ has a uniform distribution on the unit sphere in $\mathbb{R}^3$, then $\mathbf{O} = \mathbf{M}(|r|, \mathbf{u})$ from (1) belongs to the UARS class by definition with location $\mathbf{I}_3$. Using this, it suffices to consider $n = 2$ and Lemma 1 below to prove the proposition. That is, let $\mathbf{O}_1 = \mathbf{M}(|r_1|, \mathbf{u}_1)$ and $\mathbf{O}_2 = \mathbf{M}(|r_2|, \mathbf{u}_2)$ be independent rotations defined by independent $|r_1|, |r_2|$ where the conditional distribution $\mathbf{u}_i \big| |r_i|$ is uniform on the unit sphere for $i = 1, 2$. Let $\mathbf{H}$ be uniformly distributed on $SO(3)$ (cf. Miles, 1965) and independent of $\mathbf{O}_1$ and $\mathbf{O}_2$. Then, $|r_i| = \arccos[2^{-1}(tr(\mathbf{O}_i) - 1)]$ is independent of $\mathbf{H}$, and $\mathbf{H}\mathbf{u}_i \big| |r_i| \stackrel{d}{=} \mathbf{u}_i \big| |r_i|$ is uniform on the sphere for $i = 1, 2$. We then have

$$
\begin{aligned}
\mathbf{H}^T\mathbf{O}_1\mathbf{O}_2\mathbf{H} = \mathbf{H}^T\mathbf{O}_1\mathbf{H}\mathbf{H}^T\mathbf{O}_2\mathbf{H} &= \mathbf{M}(|r_1|, \mathbf{H}\mathbf{u}_1)\mathbf{M}(|r_2|, \mathbf{H}\mathbf{u}_2) \\
&\stackrel{d}{=} \mathbf{O}(|r_1|, \mathbf{u}_1)\mathbf{O}(|r_2|, \mathbf{u}_2) = \mathbf{O}_1\mathbf{O}_2
\end{aligned}
$$

and $\mathbf{O}_1\mathbf{O}_2$ belongs to the UARS class with mean rotation $\mathbf{I}_3$ by Lemma 1 below.

Lemma 1 *Let $\mathbf{O} \in SO(3)$ be a random rotation and $\mathbf{H} \in SO(3)$ be uniformly distributed and independent of $\mathbf{O}$. Then the distribution of $\mathbf{O}$ belongs to the UARS class with central direction $\mathbf{I}_3$ if and only if $\mathbf{O} \stackrel{d}{=} \mathbf{H}^T\mathbf{O}\mathbf{H}$.*

To justify Lemma 1, note that if $\mathbf{O} = \mathbf{M}(|r|, \mathbf{u})$, then $\mathbf{H}^T\mathbf{O}\mathbf{H} = \mathbf{M}(|r|, \mathbf{H}\mathbf{u})$. For any r, $\mathbf{H}\mathbf{u}\big||r|$ is uniform on the sphere (since $\mathbf{H}$ is uniform on $SO(3)$). The distributions of $\mathbf{O}$ and $\mathbf{H}^T\mathbf{O}\mathbf{H}$ are equal if and only if those of $\mathbf{H}\mathbf{u}\big||r|$ and $\mathbf{u}\big||r|$ are equal, which occurs if and only if $\mathbf{O}$ belongs to the UARS class.

S3 Evidence against the isotropic Matrix Fisher family being closed under convolution

Regarding S^{p-1}, the unit sphere in $\mathbb{R}^p$, it is known that that the set of von Mises-Fisher distributions on the sphere is not closed under convolution (Schaeben & Nikolayev, 1998, p. 78). To the best of our knowledge, there is no formal result establishing a similar fact for isotropic Matrix Fisher (IMF) distributions on $SO(3)$ but we suspect this family is also not closed under convolution. In the following, we provide numerical evidence against this family being closed.

If a random angle $r \in (-\pi, \pi]$ follows the angular density of an IMF rotation with concentration parameter $\kappa_F > 0$ (see Table 1 and Section 2.1), then

$$\mathrm{E}_{\kappa_F} \cos r = -1 + \frac{I_1(\kappa_F^2)}{\kappa_F^2[I_0(\kappa_F^2) - I_1(\kappa_F^2)]} \equiv a(\kappa_F^2), \tag{S3.1}$$

holds by simple integration, where $I_i(\cdot)$, $i = 0, 1$, denotes the modified Bessel function of order i. Additionally, if $r_1, r_2 \in (-\pi, \pi]$ are two iid draws from the angular density of an IMF rotation with concentration parameter $\kappa > 0$, and independently $\mathbf{u}_1, \mathbf{u}_2 \in \mathbb{R}^3$ are two iid vectors uniformly distributed on the $\mathbb{R}^3$ unit sphere S^2, then $\mathbf{M}(r_1, \mathbf{u}_1)$ and $\mathbf{M}(r_2, \mathbf{u}_2)$ are iid IMF rotations on $SO(3)$ with mean rotation $\mathbf{I}_3$ under the UARS construction (cf. Section 2.1 and Section S2) and their product $\mathbf{M}(r_1, \mathbf{u}_1) \cdot \mathbf{M}(r_2, \mathbf{u}_2) = \mathbf{M}(p, \mathbf{u})$ must have a UARS distribution by Lemma 1, Section S2; that is, $p \in (-\pi, \pi]$ is a random angle independent of $\mathbf{u} \in \mathbb{R}^3$ uniformly distributed on S^2. It is straightforward to check that

$$\mathrm{E}_{\kappa} \cos p = [a(\kappa^2)]^2 - \frac{1}{3}\{1 - a(\kappa^2)\}^2 \equiv b(\kappa^2) \tag{S3.2}$$

must hold, using $a(\cdot)$ from (S3.1). For $x \in (0, \infty)$, both $a(x)$ and $b(x)$ are monotonically increasing functions with range $(-0.5, 1)$, where $-0.5 = \lim_{x\to 0} a(x)$ is the expected value of $\cos r$ for an angle r associated with the uniform rotation on $SO(3)$ (i.e., an angle having Lebesgue density $g(r) = (1 - \cos r)/(2\pi)$, $r \in (\pi, \pi])$) and $1 = \lim_{x\to\infty} a(x)$ is the expected value of $\cos r$ for an angle r with a degenerate distribution at 0. If the composition $\mathbf{M}(r_1, \mathbf{u}_1) \cdot \mathbf{M}(r_2, \mathbf{u}_2) = \mathbf{M}(p, \mathbf{u})$ did indeed follow an IMF distribution on $SO(3)$ (i.e., if the IMF family was closed) regardless of the concentration parameter κ of r_1, r_2, then p would necessarily have an angular density for an IMF rotation with some unique concentration parameter $\kappa_F > 0$ (depending on κ) such that

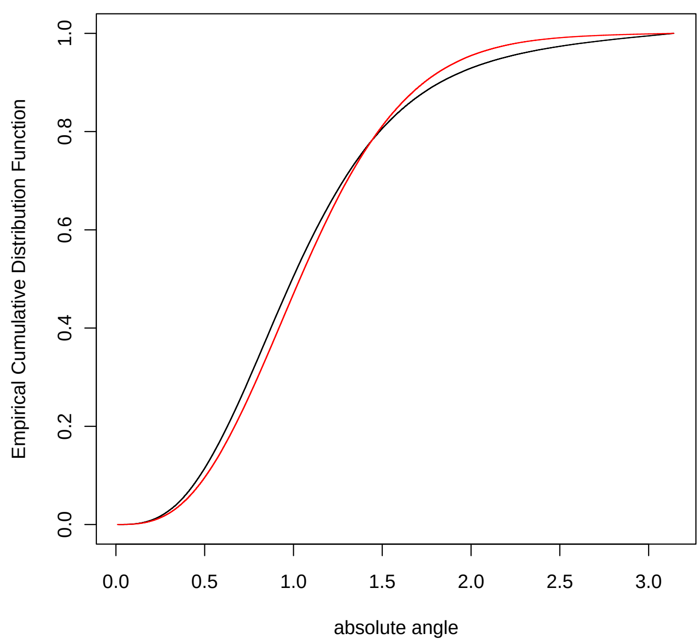
$$a(\kappa_F^2) = b(\kappa^2). \tag{S3.3}$$

However, simulation shows that the above does not hold for p having an angular density for an IMF rotation.

For instance, consider two angles r_1, r_2 as above having concentration parameter $\kappa = \sqrt{5}$. Then, if angle p from the associated matrix composition followed an angular density for an IMF rotation, its concentration parameter would need to be $\kappa_F = \sqrt{3.004183}$, solving (S3.3) as $b(5) = a(3.004183) = 0.4217894$. We generated 1,000,000 iid pairs of angles r_1, r_2 from the IMF angular density with parameter $\kappa = \sqrt{5}$

and obtained 1,000,000 realizations of $|p_i| = \arccos\{(tr[\mathbf{M}(r_1, \mathbf{u}_1) \cdot \mathbf{M}(r_2, \mathbf{u}_2)] - 1)/2\}$. We also generated 1,000,000 angles t_i from an IMF angular density with parameter $\kappa_F = \sqrt{3.004183}$. Recall the IMF angular density is symmetric around zero so that it suffices to compare the empirical distributions of $|p_i|$ and $|t_i|$ on $[0, \pi]$. From 1,000,000 simulations, the average values of $\cos|p_i|$ and $\cos|t_i|$ matched the theoretical expectations $b(5) = a(3.004183) = 0.4217894$ to five decimal places; a two sample t-test of the means of $\cos|p_i|$ and $\cos|t_i|$ gave a p-value of 0.46. Also, the averages of $|p_i|$ and $|t_i|$ matched to three decimal places with a two sample t-test giving a p-value of 0.21. However, a Mann-Whitney test for the equality of the distributions of $|p_i|$ and $|t_i|$ produced a p-value$< 10^{-16}$ and the Kolmogorov-Smirnov statistic was 0.0387 with a p-value$< 10^{-16}$. Repeating the simulations consistently produced similar results where the averages of $\cos p_i$ and $\cos t_i$ closely agreed but the empirical distributions of $|p_i|$ and $|t_i|$ differed by about 4% in places (agreeing with the Kolmogorov-Smirnov statistic), as shown in the figure below. This is again numerical evidence that the isotropic Matrix Fisher family on $SO(3)$ is not closed under convolution.

Figure 1: Empirical cumulative distribution functions for absolute angles based on 1,000,000 simulations. The red curve corresponds to the empirical distribution of $|p|$ from the product of two IMF rotations with concentration parameter $\kappa = \sqrt{5}$; the black curve corresponds to the empirical distribution of $|t|$, where t has angular density from an IMF rotation with concentration parameter $\kappa_F = \sqrt{3.004183}$. The curves should match if p has an angular density for an IFM rotation.



S4 Domain-specific conventions for expressing UARS-rotation densities

Suppose $\mathbf{O} = \mathbf{M}(r, \mathbf{u})$ denotes a random rotation resulting from the UARS construction (1) with location parameter $\mathbf{S} = \mathbf{I}_3$ and a random spin r based on an angular density $g(r|\kappa)$, $r \in (-\pi, \pi]$ (with respect to the Lesbesgue measure), symmetric around zero with concentration parameter $\kappa > 0$. From Section 2.1, recall that rotation $\mathbf{O}$ has a density with respect to the uniform distribution on $SO(3)$ given by

$$f(\mathbf{O}|\kappa) = \frac{4\pi}{3 - tr(\mathbf{O})} g(\arccos[2^{-1}(tr(\mathbf{O}) - 1)]|\kappa), \quad \mathbf{O} \in SO(3). \tag{S4.4}$$

From (1), we have the relationships $tr(\mathbf{O}) = 1 + 2\cos(r)$ and $|r| = \arccos[2^{-1}(tr(\mathbf{O}) - 1)]$ which then can be used to go back and forth, equivalently, between $f(\mathbf{O}|\kappa)$ and $g(r|\kappa)$.

In this paper, we represent rotational distributions from the UARS class in terms of their angular densities $g(r|\kappa)$, $r \in (-\pi, \pi]$ (see, for example, Table 1). However, in the material science literature, it is common (cf. Matthies et al., 1988; Nikolayev & Savyolova, 1997) to display probability densities graphically as

$$h(r|\kappa) = \frac{2\pi}{1 - \cos r} g(r|\kappa), \quad r \in (0, \pi], \tag{S4.5}$$

which expresses the *rotational* density (S4.4) as a function of the Euler angle r. In the texture analysis literature, $|r|$ is often referred to as a misorientation angle in the Euler axis-angle representation of a rotation $\mathbf{O} = \mathbf{M}(r, \mathbf{u}) = \mathbf{M}(|r|, \text{sign}(r)\mathbf{u})$ (see Section 6). Note that $|r|$ has density $2g(r|\kappa)$ on $(0, \pi]$ while the misorientation angle from the uniform distribution on $SO(3)$ has density $(1 - \cos r)/\pi$, $r \in (0, \pi]$. That is, (S4.5) is a ratio for comparing misorientation angles densities from a UARS model to the uniform model on $SO(3)$. However, the function in (S4.5) is *not* a probability density on $(0, \pi]$ and, to avoid confusion, we have elected to frame our exposition in terms of Euler angle densities on $(-\pi, \pi]$.