Frame theory in directional statistics

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Abstract

Distinguishing between uniform and non-uniform sample distributions is a common problem in directional data analysis; however for many tests, non-uniform distributions exist that fail uniformity rejection. By merging directional statistics with frame theory, we find that probabilistic tight frames yield non-uniform distributions that minimize directional potentials, leading to failure of uniformity rejection for the Bingham test. Finally, we apply our results to model patterns found in granular rod experiments.

Keywords: frames, directional statistics, Bingham test, granular rods

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1. Introduction

Observations that inherit a direction occur in many scientific disciplines. For example, directional data arise naturally in the biomedical field for protein structure, cell-cycle, and circadian clock experiments (Boomsma et al., 2008; Chassé and Théron, 1988; Levine et al., 2002; Mardia and Jupp, 2008; Mardia and Taylor, 2007; Rueda et al., 2009). Further examples occur in statistical mechanics, where experiments containing only rod-shaped particles can develop complex directional ordering (Galanis et al., 2006, 2010; de Gennes and Prost, 1993; Onsager, 1949). A simple pattern change for rod shaped objects is the density-dependent, order-disorder phase transition (de Gennes and Prost, 1993; Onsager, 1949) shown for macroscopic granular rod experiments (Galanis et al., 2006) in Fig. 1(a) and 1(b). Quantification of this transition relies on a principle component analysis (PCA) type measure that is linked with statistical

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mechanical theories (de Gennes and Prost, 1993). When applied to experimental samples whose rod orientations shift from uniform to unidirectional, this measure finds the dominant direction (director) and strength of rod ordering (order parameter).

In reality, however, experimental rod orientations are rarely unidirectional, and spatial distortions in the director field frequently occur. These distortions may result from fluctuations and/or other competing forces, like those exerted by the container boundaries in Fig. 1(c) and 1(d). Accurately quantifying rod orientations can, in fact, yield information about the collective behavior of rods, for example elastic properties (Galazis et al., 2010; de Gennes and Prost, 1993). While accurate orientation measurements of molecular-sized rods require special techniques (Hudson and Thomas, 1989), recent advances in single molecule detection may make such measurements more widely accessible (Chang et al., 2010; Xiao et al., 2010). For example, “labeled” rods can be inserted into various environments and serve as local directional sensors by aligning with the rod-shaped material around them. This technique can in principle be used in environments as complicated as a cell (Chang et al., 2010; Xiao et al., 2010) and potentially uncover intricate patterns that require more sophisticated measures of directional order.

The resulting complex patterning may reduce the value of the order parameter, sometimes to the point that the sample is inaccurately classified as disordered, Fig. 1(d). To predict which multidirectional patterns cause such misclassifications, we merge directional statistics with frame theory. Frames have proven useful in fields like spherical codes, compressed sensing, signal processing, and wavelet analysis (Casazza and Kovacevic, 2003; Christensen, 2003; Daubechies et al., 1986; Ehler, 2007, 2009, 2010a; Ehler and Han, 2008; Ehler and Koch, 2010; Feichtinger and Strohmer, 2003; Gröchenig, 2001). A frame is a basis-like system that spans a vector space but allows for linear dependency, which can be used to reduce noise, find sparse representations, or obtain other desirable features unavailable with orthonormal bases. Tight frames even provide a Parseval type formula similar to orthonormal bases. Moreover, the frame concept has recently been generalized to probability distributions on the unit sphere (Ehler, 2010b).

To analyze granular rod patterning, we consider statistical testing for directional uniformity, focusing on the Bingham test. We characterize non-uniform sample distributions that lead to failure of rejection and find that these distributions are probabilistic tight frames. Since these frames are well-understood in terms of algebraic/geometric conditions (Ehler, 2010b), further synergistic effects may develop between directional statistics and frame theory.
2. Directional statistics

Common tests in directional statistics focus on whether or not a sample on the unit sphere $S^{d-1} = \{ x \in \mathbb{R}^d : \| x \| = 1 \}$ is uniformly distributed. Here, we concentrate on two elementary tests for uniformity, Rayleigh and Bingham. Given a discrete sample $\{ x_i \}_{i=1}^n \subset S^{d-1}$, we follow the textbook (Mardia and Jupp, 2008) and define the mean as

$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i, \quad (1)$$

where the polar representation $\bar{x} = \bar{r}\bar{x}_0$ splits the mean into a mean direction $\bar{x}_0 \in S^{d-1}$ and a mean resultant length $\bar{r} = \| \bar{x} \|$. The Rayleigh test rejects the hypothesis of uniformity if $\bar{r}$ is large. More precisely, the asymptotic large-sample distribution of $dn\bar{r}^2$ under uniformity is $\chi^2_d$ distributed with an error $O(n^{-1})$, while the modified Rayleigh statistic $(1 - \frac{1}{2n})dn\bar{r}^2 + \frac{1}{2n(d+2)}d^2n^{-1}r^4$ is $\chi^2_d$ distributed with an error $O(n^{-2})$ (Mardia and Jupp, 2008).

To describe the Bingham test, let $\sigma$ denote the uniform probability measure on the sphere with respect to the Borel sigma algebra $\mathcal{B}$. We first observe that the second moments of $\sigma$ satisfy

$$M_{i,j}(\sigma) := \int_{S^{d-1}} x^{(i)}x^{(j)}d\sigma(x) = \frac{1}{d}\delta_{i,j},$$

where $x = (x^{(1)}, \ldots, x^{(d)})^\top \in \mathbb{R}^d$ and $i, j = 1, \ldots, d$. Note that the Fisher (or scatter) matrix,

$$T_{\{x_i\}_{i=1}^n} = \frac{1}{n} \sum_{i=1}^n x_i x_i^\top,$$

of a sample $\{ x_i \}_{i=1}^n \subset S^{d-1}$ equals the matrix of second moments of the underlying counting measure. Recalling that the matrix of second moments of the uniform measure equals $\frac{1}{d}\mathcal{I}_d$, the Bingham test rejects the hypothesis of directional uniformity of a sample if its Fisher matrix $T_{\{x_i\}_{i=1}^n}$ is far from $\frac{1}{d}\mathcal{I}_d$. In fact, the Bingham statistic $\frac{d(d+2)}{2}n(\text{trace}(T_{\{x_i\}_{i=1}^n}^2) - \frac{1}{d})$ under uniformity is $\chi^2_{(d-1)(d+2)/2}$ distributed with an error $O(n^{-1})$ (Mardia and Jupp, 2008).

We say that the Bingham test is inconsistent when rejection of uniformity fails for a particular non-uniform sample distribution. Here, we focus on those distributions that are multi-modal, where a mode is a local maximum of the distribution’s density. Other analysis tools have been customized to spherical and more general manifold data in Fletcher et al. (2004); Huckemann and Ziezold (2006); Jung et al. (2010).
3. Frames

A collection of points \( \{x_i\}_{i=1}^n \subset \mathbb{R}^d \) is called a finite frame for \( \mathbb{R}^d \) if there are two constants \( 0 < A \leq B \), called lower and upper frame bounds, respectively, such that

\[
A \|x\|^2 \leq \sum_{i=1}^{n} |\langle x, x_i \rangle|^2 \leq B \|x\|^2,
\]

for all \( x \in \mathbb{R}^d \), where \( \langle \cdot, \cdot \rangle \) denotes the usual inner product on \( \mathbb{R}^d \). A frame spans \( \mathbb{R}^d \), and any finite spanning set is a frame (Christensen, 2003). A collection of points \( \{x_i\}_{i=1}^n \subset \mathbb{R}^d \) is called a finite tight frame for \( \mathbb{R}^d \) if there is a positive constant \( A \), such that

\[
A \|x\|^2 = \sum_{i=1}^{n} |\langle x, x_i \rangle|^2,
\]

for all \( x \in \mathbb{R}^d \).

Every finite tight frame gives rise to the expansion

\[
x = \frac{1}{A} \sum_{i=1}^{n} \langle x, x_i \rangle x_i,
\]

for all \( x \in \mathbb{R}^d \),

which generalizes the Parseval formula for othonormal bases (Christensen, 2003).

We define a finite unit norm tight frame (FNTF) for \( \mathbb{R}^d \) as a tight frame whose elements all have unit norm. According to Goyal et al. (1998), the tight frame bound \( A \) of a FNTF is \( n/d \). The collection \( \{x_i\}_{i=1}^n \subset S^{d-1} \) is a FNTF iff its Fisher matrix equals \( \frac{1}{d} I_d \) (Christensen, 2003). The literature contains many FNTFs. For example, Sustik et al. (2007) shows a FNTF for \( \mathbb{R}^3 \) composed of 6 vectors, and \( \{(\cos(\alpha_k), \sin(\alpha_k))^T : k = 1, \ldots, n\} \) is a FNTF for \( \mathbb{R}^2 \) iff \( \sum_{k=1}^{n} e^{2i\alpha_k} = 0 \) (Goyal et al., 2001). In fact, any set of \( m \) unit norm vectors in \( \mathbb{R}^d \) can be converted to a FNTF by adding \( m(d-1) \) extra vectors (Casazza and Kovacevic, 2003).

We recall probabilistic frames as introduced in Ehler (2010b). Let \( \mathcal{M}(\mathcal{B}, S^{d-1}) \) denote the collection of probability measures on the sphere with respect to the Borel sigma algebra \( \mathcal{B} \). An element \( \mu \in \mathcal{M}(\mathcal{B}, S^{d-1}) \) is called a probabilistic unit norm frame for \( \mathbb{R}^d \) if there are constants \( 0 < A \leq B \) such that

\[
A \|x\|^2 \leq \int_{S^{d-1}} |\langle x, y \rangle|^2 d\mu(y) \leq B \|x\|^2,
\]

for all \( x \in \mathbb{R}^d \).

If we can choose \( A = B \) in (3), then we call \( \mu \) a probabilistic unit norm tight frame for \( \mathbb{R}^d \), and \( A \) must be equal to \( \frac{1}{d} \) (Ehler, 2010b). We then have

\[
x = d \int_{S^{d-1}} \langle x, y \rangle y d\mu(y), \quad \text{for all } x \in \mathbb{R}^d,
\]
where the integral is vector valued. This generalizes (2), and a sequence of pairwise distinct vectors \( \{x_i\}_{i=1}^n \subset S^{d-1} \) is a FNTF for \( \mathbb{R}^d \) iff the normalized counting measure \( \frac{1}{n} \mu_{x_1, \ldots, x_n} \) is a probabilistic unit norm tight frame for \( \mathbb{R}^d \).

4. Joining frame theory and directional statistics

As introduced in Section 2, the Rayleigh test rejects uniformity if the mean resultant length is far from 0, while the Bingham test rejects uniformity if the sample’s Fisher matrix is far from \( \frac{1}{d} I_d \). We therefore call a probability measure \( \mu \) on the sphere a Rayleigh-alternative if its mean \( \bar{\mu} = \int_{S^{d-1}} x d\mu(x) \) is 0 and a Bingham-alternative if \( M_{i,j}(\mu) = \frac{1}{2} \delta_{i,j} \) for all \( i, j = 1, \ldots, d \). We first characterize Rayleigh- and Bingham-alternatives in terms of maximizers and minimizers, respectively, of certain potentials. Subsequently, we provide a connection to probabilistic frames.

Bjoerck (1955) verifies that, among all probability measures \( \mu \in \mathcal{M}(\mathcal{B}, S^{d-1}) \), the maximizers of the probabilistic Riesz-2-potential

\[
\int_{S^{d-1}} \int_{S^{d-1}} \|x - y\|^2 d\mu(x) d\mu(y)
\]  

(4)

are exactly the zero mean probability measures. Therefore, the maximizers of (4) are the Rayleigh-alternatives.

To characterize Bingham-alternatives, we introduce the directional force \( F \) between two points \( a \) and \( b \) on the sphere \( S^{d-1} \) as \( F(a, b) = 2|\langle a, b \rangle| (a - b) \). The physical potential between \( a \) and \( b \) is \( |\langle a, b \rangle|^2 \) (Benedetto and Fickus, 2003). The minimizers of the probabilistic frame potential

\[
PFP(\mu) = \int_{S^{d-1}} \int_{S^{d-1}} |\langle x, y \rangle|^2 d\mu(x) d\mu(y),
\]  

(5)

among all probability measures \( \mu \in \mathcal{M}(\mathcal{B}, S^{d-1}) \), are said to be in equilibrium under the directional force, or simply in directional equilibrium (Benedetto and Fickus, 2003; Ehler, 2010b). Naturally, the uniform distribution is in directional equilibrium (Ehler, 2010b); however, other distributions with a mixture of well-defined modes can also be in directional equilibrium. In fact, the minimizers of the directional potential (5) are exactly those probability measures \( \mu \in \mathcal{M}(\mathcal{B}, S^{d-1}) \) whose second moments satisfy \( M_{i,j}(\mu) = \delta_{i,j} \frac{1}{d} \) (Ehler, 2010b) and are, therefore, the Bingham-alternatives. These minimizers were characterized as the probabilistic unit norm tight frames for \( \mathbb{R}^d \) in Ehler (2010b). The advantage of the latter characterization is that tight frames are well-understood in terms of algebraic as well as geometric conditions (Benedetto and Fickus, 2003; Christensen, 2003; Ehler, 2010b).

Results in Ehler (2010b) and the present work imply that the Bingham-
alternatives with zero mean are the minimizers of the fractional frame-Riesz-2-potential
\[ \int_{S^{d-1}} \int_{S^{d-1}} |\langle x, y \rangle|^2 d\mu(x) d\mu(y) / \int_{S^{d-1}} \int_{S^{d-1}} \|x - y\|^2 d\mu(x) d\mu(y). \] (6)

Hence, probabilistic unit norm tight frames with zero mean are both, Rayleigh- and Bingham-alternatives.

5. Patterning of granular rods

5.1. Order-disorder phase transition

A collection of rod shaped particles can undergo an order-disorder phase transition that, in the simplest model, is controlled by entropy. At low rod densities, the maximal total entropy occurs when both rotational and translational entropies are independently maximized. Beyond a critical density, however, rotational entropy is sacrificed for significant gains in translational entropy, resulting in a phase transition from randomly (uniformly) rotated rods, Fig. 1(a), to directionally oriented rods, Fig. 1(b). A PCA-type method measures the average rod direction (director) and strength of rod alignment (order parameter) that results from rotational entropy loss and is described in the following: Let \( x_i \in S^{d-1} \) denote the direction of the \( i \)-th rod out of \( n \) total rods. For simplicity, let us assume that the alignment is measured in a plane, hence \( d = 2 \). The covariance type matrix
\[ Q_2 = \frac{1}{n} \sum_{i=1}^{n} 2x_i x_i^\top - I_2 \] (7)
is therefore used to determine the director. Since \( Q_2 \) is symmetric, the eigenvectors form an orthogonal basis, where the nonnegative eigenvalue \( \lambda \) corresponds to the order parameter and the associated eigenvector corresponds to the director, cf. Frenkel and Eppenga (1985); Galanis et al. (2006). In fact, \( 0 \leq \lambda \leq 1 \) and the second eigenvalue of \( Q_2 \) equals \(-\lambda\).

This PCA-type method only measures unidirectional rod ordering. In experiments, however, fluctuations and/or competing forces like container boundaries, Figs. 1(c) and 1(d), can influence rod alignment. Therefore, the director field can vary spatially, potentially resulting in complex multidirectional patterning, Fig. 1(d), that sometimes cannot be distinguished from a disordered state when analyzed by the traditional order parameter.

5.2. New model by means of directional statistics

We propose a complementary analysis of rod ordering that can more accurately quantify multidirectional alignment. We fit a probability model to experimentally observed rod patterning by first identifying a set of directions, cf. Fig. 1(b)-(d). Since a rod rotated by 180 degrees is indistinguishable from an
Figure 1: Rod patterns observed in 2D. (top) Images from granular rod experiments showing a disordered state (a), unidirectional ordered states with small (b) and large (c) standard deviations, and a multidirectional ordered state (d). The order parameters derived from $Q_2$ in (7) are $0.0950$ (a), $0.8902$ (b), $0.4267$ (c), and $0.1534$ (d). The Bingham test rejects uniformity at a 1% confidence level for (b) and (c); however, uniformity cannot be rejected at a 5% confidence level for (a) and (d). Color represents the local order parameter, where $Q_2$ is measured only in a vicinity of less than one rod length from each location in the image. (center) Directional histograms (blue) and directors $z_i$ (dashed red lines) associated with each state. (bottom) We apply the Watson mixture model in (9) with a suitable $\kappa$.

unrotated rod, we do not differentiate between $x$ and $-x$. Consistent with this criteria, let $\sigma \in \mathcal{M}(B, S^{d-1})$ be the uniform measure on the sphere, $z_0 \in S^{d-1}$, and $\kappa \neq 0$, the Watson measure $\mu$ is then given by

$$
\mu(x) = c_d(\kappa) \exp(\kappa(z_0, x)^2)\sigma(x),
$$

where $c_d(\kappa) = \frac{\Gamma(d/2)}{2\pi^{d/2} F(1/2, d/2, \kappa)}$, $\Gamma$ the usual Gamma function, and $F$ a confluent hypergeometric function (Mardia and Jupp, 2008). For $\kappa > 0$, the density tends to concentrate around $\pm z_0$, whereas for $\kappa < 0$, the density concentrates around the great circle orthogonal to $z_0$. And as $|\kappa|$ increases, the density peaks tighten.

Next, we model each sample with a mixture of Watson distributions, i.e.,
for a collection of directors \( \{z_i\}_{i=1}^N \subset S^1 \), we consider
\[
\mu(x) = \frac{c_2(\kappa)}{N} \sum_{i=1}^{N} \exp(\kappa \langle z_i, x \rangle^2) \sigma(x).
\tag{9}
\]

If \( \{z_i\}_{i=1}^N \) is a FNTF for \( \mathbb{R}^2 \), then, for any \( \kappa \neq 0 \), the measure (9) is a probabilistic unit norm tight frame for \( \mathbb{R}^2 \) (Ehler, 2010b), hence a Bingham-alternative. Note that in \( \mathbb{R}^2 \), a FNTF with three elements (directions) must be equiangular, and all equiangular tri-directions are FNTFs (Goyal et al., 2001). Nevertheless, if a sample is distributed so that the modes in (9) approximate a minimizer, like the three nearly equiangular directions in Fig. 1(d), then the Bingham test may also fail to reject uniformity, as is the case with this figure.

Finally, this approach extracts two parameter sets from the sample, directional modes and associated widths (Bartels, 1984; Fisher, 1995; Hsu et al., 1986), where the widths represent a measure for directional ordering. These parameters will be used in a forthcoming paper to quantify the differences between experimental rod patterns and the expected behavior from theories and simulations. Furthermore, these tools may provide a method to identify more subtle rod patterning transitions, like the one described in Galanis et al. (2010).

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