Statistics of ambiguous rotations

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Abstract

The orientation of a rigid object can be described by a rotation that transforms it into a standard position. For a symmetrical object the rotation is known only up to multiplication by an element of the symmetry group. Such ambiguous rotations arise in biomechanics, crystallography and seismology. We develop methods for analyzing data of this form. A test of uniformity is given. Parametric models for ambiguous rotations are presented, tests of location are considered, and a regression model is proposed. A brief illustrative example involving orientations of diopside crystals is given.

Keywords: Frame, Orientation, Regression, Symmetry, Tensor, Test of uniformity.

1 Introduction

Data that are rotations of \mathbb{R}^3 occur in various areas of science, such as palaeo-magnetism (Pesonen et al., 2003; Villalaín et al., 2016; Koymans et al., 2016), plate tectonics and seismology (Stein & Wysession, 2003; Hardebeck, 2006; Arnold & Townend, 2007; Walsh et al., 2009; Khalil & McClay, 2016), biomechanics (Rivest, 2005; Lekadir et al., 2015; Spronck et al., 2016), crystallography (Hielscher et al., 2010; Griffiths et al., 2016) and texture analysis, i.e., analysis of orientations of crystalites (Kunze & Schaeben, 2004, 2005; Du et al., 2016). The sample space is the 3-dimensional rotation group, SO(3), and methods for handling such data are now an established

part of directional statistics; see §13.2 of Mardia & Jupp (2000). In some contexts the presence of symmetry means that the rotations are observed subject to ambiguity, so that it is not possible to distinguish a rotation X from **XR** for any rotation **R** in some given subgroup K of SO(3). From the mathematical point of view, the sample space is the quotient SO(3)/Kof SO(3) by K. Such spaces arise in many scientific contexts: the case in which K is generated by the rotations through 180° about the coordinate axes gives the orthogonal axial frames considered by Arnold & Jupp (2013), which can be used to describe aspects of earthquakes; many groups K of low order occur as the symmetry groups of crystals; the icosahedral group is the symmetry group of some carborane molecules (Jemmis, 1982), of most closed-shell viruses (Harrison, 2013), of the natural quasicrystal, icosahedrite (Bindi et al., 2011), and of the blue phases of some liquid crystals (Seideman, 1990, §6.1.2). The object of this paper is to give a unified account of some general tools for the analysis of data consisting of ambiguous rotations with a finite symmetry group.

2 Ambiguous rotations

2.1 Symmetry groups

The orientation of a rigid object in \mathbb{R}^3 can be described by a rotation that transforms it into some standard position. If the object is asymmetrical then this rotation is unique, so that the orientations of the object correspond to elements of the rotation group SO(3). If the object is symmetrical then the set of rotations that have no visible effect on the object forms a subgroup K of SO(3). Then the orientations of the object correspond to elements of the homogeneous space SO(3)/K, i.e. the set of equivalence classes of elements of SO(3) under the right action of K. We shall consider the cases in which K is finite. In particular, the orientations of T-shaped, X-shaped and +-shaped objects in \mathbb{R}^3 are elements of SO(3)/K with $K = C_2, D_2$ and D_4 , respectively. For U in SO(3) we shall denote the equivalence class of U in SO(3)/K by [U].

The finite subgroups of SO(3) are known also as the point groups of the first kind. The classification result for these groups, given e.g. in Miller (1972), states that any such group is isomorphic to one of the following: the cyclic groups, C_r , for r = 1, 2, ..., the dihedral groups, D_r , for r = 2, 3, ..., the tetrahedral group, T, the octahedral group, O, and the icosahedral group, Y. These groups are listed in Table 1, together with the frames of vectors that will be used to represent elements of the sample spaces SO(3)/K.

The group C_1 has one element, the identity, I_3 .

2.2 Frames and symmetric frames

For each point group K of the first kind, every element of SO(3)/K can be represented uniquely by a K-frame, i.e. an equivalence class of a frame, meaning a set of vectors or axes in \mathbb{R}^3 . For $K=C_r$ with $r\geq 3$ or $K=D_r$ with $r\geq 3$, it is convenient to take the vectors of the frame to be unit normals to the sides of a regular r-gon; for $K=C_2$ we take a unit vector and an axis orthogonal to it; for $K=D_2$ we take a pair of orthogonal axes; for K=T,O or Y, it is convenient to take the vectors to be unit normals to the sides of a regular tetrahedron, cube or dodecahedron, respectively. Permutation of the vectors of the frame by the action of K leads to ambiguity. This ambiguity is removed by passing to the corresponding K-frame, i.e. the equivalence class of the frame under such permutations. The K-frames will be denoted by square brackets, e.g. for $K=C_r$, $[\mathbf{u}_1,\ldots,\mathbf{u}_r]$ denotes the K-frame arising from $(\mathbf{u}_1,\ldots,\mathbf{u}_r)$. By a symmetric frame, we shall mean a K-frame for some K. The frames that we consider are listed in Table 1, together with an indication of the ambiguities.

Table 1: Symmetry groups and frames.

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Group	Name	Frame		
C_1	trivial	$({f u}_1,{f u}_2,{f u}_3)$	$\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3$ orthonormal, $\mathbf{u}_3 = \mathbf{u}_1 \times \mathbf{u}_2$	
C_2	cyclic	$(\mathbf{u}_0,\pm\mathbf{u}_1)$	$\mathbf{u}_0, \mathbf{u}_1$ orthonormal	
$C_r (r \ge 3)$	cyclic	$(\mathbf{u}_1,\ldots,\mathbf{u}_r)$	$\mathbf{u}_1, \dots, \mathbf{u}_r$ coplanar,	
			known up to cyclic order,	
			$\mathbf{u}_i^{\mathrm{T}}\mathbf{u}_{i-1} = \cos(2\pi/r) \text{ for } i = 2, \dots, r$	
D_2	dihedral	$(\pm \mathbf{u}_1, \pm \mathbf{u}_2)$	orthogonal axes	
$D_r (r \ge 3)$	dihedral	$(\mathbf{u}_1,\ldots,\mathbf{u}_r)$	$\mathbf{u}_1, \dots, \mathbf{u}_r$ coplanar,	
			known up to cyclic order and reversal,	
			$\mathbf{u}_{i}^{\mathrm{T}}\mathbf{u}_{i-1} = \cos(2\pi/r) \text{ for } i = 2, \dots, r$	
$T = A_4$	tetrahedral	$\{\mathbf{u}_1,\ldots,\mathbf{u}_4\}$	$\mathbf{u}_{i}^{\mathrm{T}}\mathbf{u}_{j} = -1/3 \text{ for } i \neq j$	
$O = \Sigma_4$	octahedral	$\{\pm \mathbf{u}_1, \pm \mathbf{u}_2, \pm \mathbf{u}_3\}$	orthogonal axes	
	= cubic			
$Y = A_5$	icosahedral	$\{\pm \mathbf{u}_1,\ldots,\pm \mathbf{u}_6\}$	$ \mathbf{u}_i^{\mathrm{T}}\mathbf{u}_i = 5^{-1/2} \text{ for } i \neq j$	
	$= {\rm dodecahedral} \\$			

The \mathbf{u}_i are unit vectors.

Special cases of Table 1 include the 7 crystal systems: triclinic, monoclinic, trigonal, tetragonal, orthorhombic, hexagonal and cubic with symmetry groups C_1 , C_2 , C_3 , C_4 , D_2 , D_6 and O, respectively.

3 Transforming symmetric frames to tensors

3.1 Embeddings of the sample spaces

In order to carry out statistics on SO(3)/K, we shall take the embedding approach used in, e.g. §10.8 of Mardia & Jupp (2000). We shall embed SO(3)/K in an inner-product space, E, on which SO(3) acts. The embedding will be a well-defined equivariant one-to-one function $\mathbf{t}: SO(3)/K \to$ E such that $\mathbf{t}([\mathbf{U}])$ has expectation $\mathbf{0}$ if $[\mathbf{U}]$ is uniformly distributed on SO(3)/K. For $E=L^2(SO(3))$, the space of square-integrable functions on SO(3), a very wide class of such embeddings can be obtained by averaging over K. Let $\mathbf{t}_0: SO(3) \to L^2(SO(3))$ be an embedding used in the Hilbert space approach to Sobolev tests of uniformity; see §§10.8, 13.2.2 of Mardia & Jupp (2000), Giné (1975) and §4 of Prentice (1978). Define $\mathbf{t}: SO(3)/K \to L^2(SO(3))$ by $\mathbf{t}([\mathbf{U}]) = |K|^{-1} \sum_{\mathbf{R} \in K} \mathbf{t}_0(\mathbf{U}\mathbf{R})$, where |K|denotes the number of elements in K. If t is one-to-one then it is an embedding. In general, such t are quite complicated, so in this paper, for each K, we focus on a simple choice of embedding, \mathbf{t}_K , of SO(3)/K into an appropriate space of symmetric tensors. These \mathbf{t}_K are given in Table 2. Corresponding expressions for $\langle \mathbf{t}_K([\mathbf{U}]), \mathbf{t}_K([\mathbf{W}]) \rangle$ with $\mathbf{U}, \mathbf{W} \in SO(3)$ are given in Table 3. Here $\langle \cdot, \cdot \rangle$ is the standard inner product on the appropriate tensor product.

Table 2: Some embeddings $\mathbf{t}_K : SO(3)/K \to E$.

Group, K	\mathbf{t}_K
C_1	$\mathbf{t}_{C_1}(\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3) = (\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3)$
C_2	$\mathbf{t}_{C_2}(\mathbf{u}_0, \pm \mathbf{u}_1) = (\mathbf{u}_0, \mathbf{u}_1 \mathbf{u}_1^{\mathrm{T}} - (1/3)\mathbf{I}_3)$
$C_r (r \ge 3)$	
r odd	$\mathbf{t}_{C_r}([\mathbf{u}_1,\ldots,\mathbf{u}_r]) = \left(\mathbf{u}_0,\sum_{i=1}^r \otimes^r \mathbf{u}_i ight)$
r even	$\mathbf{t}_{C_r}([\mathbf{u}_1,\ldots,\mathbf{u}_r]) = (\mathbf{u}_0,\sum_{i=1}^r \otimes^r \mathbf{u}_i - r/(r+1)\operatorname{symm}(\otimes^{r/2}\mathbf{I}_3))$
D_2	$\mathbf{t}_{D_2}(\pm \mathbf{u}_1, \pm \mathbf{u}_2) = (\mathbf{u}_1 \mathbf{u}_1^{\mathrm{T}} - (1/3)\mathbf{I}_3, \mathbf{u}_2 \mathbf{u}_2^{\mathrm{T}} - (1/3)\mathbf{I}_3, \mathbf{u}_3 \mathbf{u}_3^{\mathrm{T}} - (1/3)\mathbf{I}_3)$
$D_r (r \ge 3)$	
r odd	$\mathbf{t}_{D_r}([\mathbf{u}_1,\ldots,\mathbf{u}_r]) = \sum_{i=1}^r \otimes^r \mathbf{u}_i$
r even	$\mathbf{t}_{D_r}([\mathbf{u}_1,\dots,\mathbf{u}_r]) = \sum_{i=1}^r \otimes^r \mathbf{u}_i - r/(r+1) \operatorname{symm}(\otimes^{r/2} \mathbf{I}_3)$ $\mathbf{t}_T(\{\mathbf{u}_1,\mathbf{u}_2,\mathbf{u}_3,\mathbf{u}_4\}) = \otimes^3 \mathbf{u}_1 + \otimes^3 \mathbf{u}_2 + \otimes^3 \mathbf{u}_3 + \otimes^3 \mathbf{u}_4$
T	$\mathbf{t}_T(\{\mathbf{u}_1,\mathbf{u}_2,\mathbf{u}_3,\mathbf{u}_4\}) = \otimes^3 \mathbf{u}_1 + \otimes^3 \mathbf{u}_2 + \otimes^3 \mathbf{u}_3 + \otimes^3 \mathbf{u}_4$
O	$\mathbf{t}_O(\{\pm \mathbf{u}_1, \pm \mathbf{u}_2, \pm \mathbf{u}_3\}) = \otimes^4 \mathbf{u}_1 + \otimes^4 \mathbf{u}_2 + \otimes^4 \mathbf{u}_3 - (3/5) \operatorname{symm}(\otimes^2 \mathbf{I}_3)$
Y	$\mathbf{t}_Y(\{\pm \mathbf{u}_1,\dots,\pm \mathbf{u}_6\}) = \sum_{i=1}^6 \otimes^{10} \mathbf{u}_i - (6/11) \operatorname{symm}(\otimes^5 \mathbf{I}_3)$

For C_r , $\mathbf{u}_0 = \{\sin(2\pi/r)\}^{-1} \mathbf{u}_1 \times \mathbf{u}_2$. For D_2 , $\mathbf{u}_3 = \pm \mathbf{u}_1 \times \mathbf{u}_2$. 'symm' denotes symmetrization over permutations of factors of the tensor product.

Define
$$\rho^2$$
 by
$$\rho^2 = \|\mathbf{t}([\mathbf{U}])\|^2, \tag{1}$$

which has the same value for all U in SO(3). Then t embeds SO(3)/K in the sphere of radius ρ with centre the origin in the vector space E.

Table 3: Inner products of transforms of symmetric frames.

Group, K	Inner product
C_1	$\langle \mathbf{t}_{C_1}(\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3), \mathbf{t}_{C_1}(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3) \rangle = \mathbf{u}_1^{\mathrm{T}} \mathbf{v}_1 + \mathbf{u}_2^{\mathrm{T}} \mathbf{v}_2 + \mathbf{u}_3^{\mathrm{T}} \mathbf{v}_3$
C_2	$\langle \mathbf{t}_{C_2}(\mathbf{u}_0, \pm \mathbf{u}_1), \mathbf{t}_{C_2}(\mathbf{v}_0, \pm \mathbf{v}_1) \rangle = \mathbf{u}_0^{\mathrm{T}} \mathbf{v}_0 + \left(\mathbf{u}_1^{\mathrm{T}} \mathbf{v}_1\right)^2 - 1/3$
$C_r (r \ge 3)$	· · · · · · · · · · · · · · · · · · ·
r odd	$\langle \mathbf{t}_{C_r}([\mathbf{u}_1,\ldots,\mathbf{u}_r]),\mathbf{t}_{C_r}([\mathbf{v}_1,\ldots,\mathbf{v}_r]) angle = \mathbf{u}_0^{\mathrm{T}}\mathbf{v}_0 + \sum_{i=1}^r \sum_{j=1}^r \left(\mathbf{u}_i^{\mathrm{T}}\mathbf{v}_j\right)^r$
r even	$\langle \mathbf{t}_{C_r}([\mathbf{u}_1,\ldots,\mathbf{u}_r]), \mathbf{t}_{C_r}([\mathbf{v}_1,\ldots,\mathbf{v}_r]) \rangle = \mathbf{u}_0^{\mathrm{T}} \mathbf{v}_0 + \sum_{i=1}^r \sum_{j=1}^r \left(\mathbf{u}_i^{\mathrm{T}} \mathbf{v}_j \right)^r - r^2/(r+1)$
D_2	$\langle \mathbf{t}_{D_2}(\pm \mathbf{u}_1, \pm \mathbf{u}_2), \mathbf{t}_{D_2} \pm \mathbf{v}_1, \pm \mathbf{v}_2) \rangle = \left(\mathbf{u}_1^{\mathrm{T}} \mathbf{v}_1\right)^2 + \left(\mathbf{u}_2^{\mathrm{T}} \mathbf{v}_2\right)^2 + \left(\mathbf{u}_3^{\mathrm{T}} \mathbf{v}_3\right)^2 - 1$
$D_r (r \ge 3)$	
r odd	$\langle \mathbf{t}_{D_r}([\mathbf{u}_1,\ldots,\mathbf{u}_r]),\underline{\mathbf{t}}_{D_r}([\mathbf{v}_1,\ldots,\mathbf{v}_r]) angle = \sum_{i=1}^r \sum_{j=1}^r \left(\mathbf{u}_i^{\mathrm{T}}\mathbf{v}_j ight)^r$
r even	$\langle \mathbf{t}_{D_r}([\mathbf{u}_1,\ldots,\mathbf{u}_r]), \mathbf{t}_{D_r}([\mathbf{v}_1,\ldots,\mathbf{v}_r]) \rangle = \sum_{i=1}^r \sum_{j=1}^r (\mathbf{u}_i^T \mathbf{v}_j)^r - r^2/(r+1)$
T	$\langle \mathbf{t}_T(\{\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3, \mathbf{u}_4\}), \mathbf{t}_T(\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \mathbf{v}_4\}) angle = \sum_{i=1}^4 \sum_{j=1}^4 \left(\mathbf{u}_i^{\mathrm{T}} \mathbf{v}_j\right)^3$
O	$\langle \mathbf{t}_O(\{\pm \mathbf{u}_1, \pm \mathbf{u}_2, \pm \mathbf{u}_3\}), \mathbf{t}_O(\{\pm \mathbf{v}_1, \pm \mathbf{v}_2, \pm \mathbf{v}_3\}) \rangle = \sum_{i=1}^3 \sum_{j=1}^3 \left(\mathbf{u}_i^{\mathrm{T}} \mathbf{v}_j\right)^4 - 9/5$
Y	$\langle \mathbf{t}_Y(\{\pm \mathbf{u}_1, \dots, \pm \mathbf{u}_6\}), \mathbf{t}_Y(\{\pm \mathbf{v}_1, \dots, \pm \mathbf{v}_6\}) \rangle = \sum_{i=1}^6 \sum_{j=1}^6 (\mathbf{u}_i^{\mathrm{T}} \mathbf{v}_j)^{10} - 36/11$
	For C_r , $\mathbf{u}_0 = \{\sin(2\pi/r)\}^{-1} \mathbf{u}_1 \times \mathbf{u}_2$. For D_2 , $\mathbf{u}_3 = \pm \mathbf{u}_1 \times \mathbf{u}_2$.

Each symmetric frame can be represented by an element \mathbf{U} of SO(3). In the triclinic case, where $K=C_1$, \mathbf{U} is unique and $\mathbf{t}([\mathbf{U}])=\mathbf{U}$. We have restricted our attention to point groups, K, of the first kind, i.e., excluding reflections. However, in situations where reflection symmetries are also present we can adopt a right-handed convention for all orientations, and then neglect reflections. For example, we can treat observations on $O(3)/\{\mathbf{I}_3, -\mathbf{I}_3\}$ in the same way as those on $SO(3)=SO(3)/C_1$.

3.2 Sample mean

Observations $[\mathbf{U}_1], \ldots, [\mathbf{U}_n]$ in SO(3)/K can usefully be summarized by the sample mean $\bar{\mathbf{t}}$ of their images by \mathbf{t} , i.e., by $\bar{\mathbf{t}} = n^{-1} \sum_{i=1}^{n} \mathbf{t}([\mathbf{U}_i])$. The sample mean $[\bar{\mathbf{U}}]$ is defined as the $[\mathbf{U}]$ in SO(3)/K that maximizes $\langle \mathbf{t}([\bar{\mathbf{U}}]), \bar{\mathbf{t}} \rangle$. Although $[\bar{\mathbf{U}}]$ is not necessarily unique, it follows from Theorem 3.2 of Bhattacharya & Patrangenaru (2003) that if $[\mathbf{U}_1], \ldots, [\mathbf{U}_n]$ are generated by a continuous distribution then $[\bar{\mathbf{U}}]$ is unique with probability 1.

3.3 Sample dispersion

A sensible measure of dispersion is

$$d = \rho^2 - \|\bar{\mathbf{t}}\|^2, \tag{2}$$

analogous to the quantity $1 - \bar{R}^2$ used for spherical data; see p. 164 of Mardia & Jupp (2000). The dispersion satisfies the inequalities $0 \le d \le \rho^2$, where ρ^2 is defined in (1). Since **t** is one-to-one, d = 0 if and only if $[\mathbf{U}_1] = \ldots = [\mathbf{U}_n]$. Transformation of $[\mathbf{U}_1], \ldots, [\mathbf{U}_n]$ to $[\mathbf{V}\mathbf{U}_1], \ldots, [\mathbf{V}\mathbf{U}_n]$ with **V** in SO(3) leaves d unchanged. If $K = C_1$ then $d = 3 - \operatorname{trace}(\bar{\mathbf{R}}^2)$, where $\bar{\mathbf{R}} = (\bar{\mathbf{X}}^T\bar{\mathbf{X}})^{1/2}$ with $\bar{\mathbf{X}} = \bar{\mathbf{t}}$, the sample mean of $\mathbf{X} = (\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3)$, as in p. 290 of Mardia & Jupp (2000). If $K = D_2$ then $d = d_1$, where d_1 is one of the measures of dispersion defined in §2.3 of Arnold & Jupp (2013).

4 Tests of uniformity

4.1 A simple test

The uniform distribution on SO(3)/K is the unique distribution that is invariant under the action of SO(3) on SO(3)/K in which \mathbf{V} in SO(3) maps $[\mathbf{U}]$ to $[\mathbf{V}\mathbf{U}]$. Since the embeddings \mathbf{t} were chosen so that $\mathbf{E}\{\mathbf{t}([\mathbf{U}])\}=\mathbf{0}$ for \mathbf{U} uniformly distributed on SO(3)/K, it is intuitively reasonable to reject uniformity if \mathbf{t} is far from $\mathbf{0}$, i.e. if $n\|\mathbf{t}\|^2$ is large. Significance can be assessed using simulation from the uniform distribution. For large samples, the following asymptotic result can be used.

Proposition 1

Given a random sample on SO(3)/K, define S by

$$S = (\nu/\rho^2) n \|\bar{\mathbf{t}}\|^2 = n\nu (1 - d/\rho^2), \tag{3}$$

where ρ^2 and d are given by (1) and (2), respectively, and ν is the dimension of E.

- (i) For $K = C_1, D_r$ with $r \geq 2$, T, O or Y, under uniformity, the asymptotic distribution of S is $S \sim \chi^2_{\nu}$, as $n \to \infty$.
- (ii) For $K = C_2$,

$$S = (1/3)S_R + (2/15)S_B,$$

where $S_R = 3n\bar{R}^2$ is the Rayleigh statistic for uniformity of \mathbf{u}_0 and $S_B = (15/2)n\left\{\mathrm{tr}(\bar{\mathbf{T}}^2) - (1/3)\right\}$ is the Bingham statistic for uniformity of $\pm \mathbf{u}_1$, \bar{R} being the mean resultant length of \mathbf{u}_0 and $\bar{\mathbf{T}}$ being the sample scatter matrix of $\pm \mathbf{u}_1$. Under uniformity, S_R and S_B are asymptotically independent with asymptotic distributions χ_3^2 and χ_5^2 , respectively.

(iii) For $K = C_r$ with $r \geq 3$,

$$(\nu_C/\rho_C^2)S = (1/3)S_R + (\nu_D/\rho_D^2)S_D,$$

where the subscripts C and D refer respectively to C_r -frames and the corresponding D_r -frames obtained by replacing the directed normal to the plane of a C_r -frame by the undirected normal, and $S_R = 3n\bar{R}^2$ is the Rayleigh statistic for uniformity of \mathbf{u}_0 . Under uniformity, S_R and S_D are asymptotically independent with asymptotic distributions χ_3^2 and $\chi_{\nu_D}^2$, respectively.

Values of ρ^2 and ν are given in Table 4. In the case $K = C_1$, S is the Rayleigh statistic (Mardia & Jupp, 2000, p. 287) for testing uniformity on SO(3). In the case $K = D_2$, S is the statistic given in §3 of Arnold & Jupp (2013) for testing uniformity on $O(3)/\mathbb{Z}_2^3$.

Table 4: Values of squared radius, ρ^2 , and dimension, ν

10010	raides of squared radius, p, and	, , , , , , , , , , , , , , , , , , ,
Group	$ ho^2$	u
C_1	3	9
C_2	5/3	8
$C_r (r \ge 3)$,	
r odd	$1 + 2^{1-r}r^2$	(r+2)(r+1)/2+3
r even	$1 + r^2 2^{1-r} \left\{ 1 + 2^{-1} {r \choose r/2} \right\} - r^2/(r+1)$	(r+2)(r+1)/2+3
D_2	2	10
$D_r (r \ge 3)$		
r odd	$2^{1-r}r^2$	(r+2)(r+1)/2
r even	$r^{2}2^{1-r}\left\{1+2^{-1}\binom{r}{r/2}\right\}-r^{2}/(r+1)$	(r+2)(r+1)/2
T	32/9	10
O	6/5	9
Y	18816/6875	21

4.2 Some consistent tests

The test of uniformity based on S is consistent only against alternatives for which $\mathrm{E}\{\mathbf{t}([\mathbf{U}])\}$ is non-zero. For example, in any equal mixture of two frame cardioid distributions with densities (8) having concentrations κ and $-\kappa$, $E\{\mathbf{t}([\mathbf{U}])\} = \mathbf{0}$, and so, in asymptotically large samples, S cannot distinguish between such mixtures and the uniform distribution.

Tests of uniformity on SO(3)/K that are consistent against all alternatives can be obtained as follows by averaging over K Prentice's generalization to $\mathbb{R}P^3$ of Giné's G_n test of uniformity; see §4 of Prentice (1978) and §13.2.2 of Mardia & Jupp (2000). Given $[\mathbf{U}_1], \ldots, [\mathbf{U}_n]$ in SO(3)/K, with representatives $\mathbf{U}_1, \ldots, \mathbf{U}_n$ in SO(3), put

$$T_G = -\sum_{i=1}^n \sum_{j=1}^n \sum_{\mathbf{R} \in K} \left\{ 3 - \operatorname{trace} \left(\mathbf{U}_i^{\mathrm{T}} \mathbf{U}_j \mathbf{R} \right) \right\}^{1/2}, \tag{4}$$

cf. the construction in §2 of Jupp & Spurr (1983). Uniformity is rejected if T_G is large compared with the randomization distribution obtained by replacing $\mathbf{U}_1, \ldots, \mathbf{U}_n$ by $\mathbf{R}_1\mathbf{U}_1, \ldots, \mathbf{R}_n\mathbf{U}_n$, where $\mathbf{R}_1, \ldots, \mathbf{R}_n$ are independent random rotations obtained from the uniform distribution on SO(3). The orthorhombic case, $K = D_2$, is considered in §3 of Arnold & Jupp (2013). It follows from Theorem 3.1 of Jupp & Spurr (1983) and the consistency of Giné's test on $\mathbb{R}P^3$ (Mardia & Jupp, 2000, p. 289) that the test based on T_G is consistent against all alternatives. More general Sobolev statistics on SO(3)/K can be obtained from Sobolev statistics on SO(3) by averaging over K, as in (4).

Permutational multi-sample tests, tests of symmetry, tests of independence, and goodness-of-fit tests for symmetric frames can be obtained by applying the machinery of Wellner (1979), Jupp & Spurr (1983), Jupp & Spurr (1985) and Jupp (2005), respectively, to the embedding \mathbf{t} . These tests of independence are considered in $\S 7$.

5 Distributions on SO(3)/K

5.1 A general class of distributions

An appealing class of distributions on SO(3)/K consists of those with densities of the form

$$f([\mathbf{U}]; [\mathbf{M}], \kappa) = g(\langle \mathbf{t}([\mathbf{U}]), \mathbf{t}([\mathbf{M}]) \rangle; \kappa),$$
 (5)

where $g(\cdot;\kappa)$ is a suitable known function and $[\mathbf{M}] \in SO(3)/K$. The parameter $[\mathbf{M}]$ measures location and κ measures concentration. If $g(\cdot;\kappa)$ is a strictly increasing function, as in (6) or León et al. (2006) with $\kappa > 0$, then the mode is $[\mathbf{M}]$.

In the case $K = C_1$, the densities (5) depend on **U** only through trace(**UM**^T) and the axes and the rotation angles of the random rotations are independent, with the axes being uniformly distributed. These distributions were

introduced by Bingham et al. (2009) under the name of uniform axis-random spin distributions and by Hielscher et al. (2010) under the name of radially symmetric distributions. For $K \neq C_1$, elements of SO(3)/K do not have well-defined axes and, in general, the distributions on SO(3) with densities \tilde{f} of the form $\tilde{f}(\mathbf{U}) = f([\mathbf{U}]; [\mathbf{M}], \kappa)$ do not have uniformly distributed axes. Taking $g(x; \kappa)$ proportional to $e^{\kappa x}$ in (5) gives the densities of the form

$$f([\mathbf{U}]; [\mathbf{M}], \kappa) = c(\kappa)^{-1} \exp\{\kappa \langle \mathbf{t}([\mathbf{U}]), \mathbf{t}([\mathbf{M}]) \rangle\}.$$
 (6)

For $\kappa > 0$, the mode is [M] and the maximum likelihood estimate of [M] is the sample mean. The family (6) is a subfamily of the crystallographic exponential family introduced by Boogaart (2002, §3.2). For $K = C_1$, (6) is the density of the matrix Fisher distribution with parameter matrix $\kappa \mathbf{M}$ and $c(\kappa) = {}_0F_1(3/2, (\kappa^2/4)\mathbf{I}_3)$ (Mardia & Jupp, 2000, §13.2.3). For $K = D_2$, (6) is the density of the equal concentration frame Watson distributions considered in Arnold & Jupp (2013, §6.1). Taking $g(x;\kappa)$ proportional to $(1+x)^{\kappa}$ in (5) gives the densities of the form

$$f([\mathbf{U}]; [\mathbf{M}], \kappa) = c(\kappa)^{-1} \left\{ 1 + \langle \mathbf{t}([\mathbf{U}]), \mathbf{t}([\mathbf{M}]) \rangle \right\}^{\kappa}.$$
 (7)

For $K = C_1$, these densities are those of the de la Vallée Poussin distributions introduced by Schaeben (1997), and, under the name of Cayley distributions, by León et al. (2006).

Taking $g(x) = 1 + \kappa x$ with $0 \le \kappa \le \rho^{-2}$ in (5) gives the densities

$$f([\mathbf{U}]; [\mathbf{M}], \kappa) = 1 + \kappa \langle \mathbf{t}([\mathbf{U}]), \mathbf{t}([\mathbf{M}]) \rangle$$
 (8)

of the frame cardioid distributions, which are analogous to the cardioid distributions on the circle (Mardia & Jupp, 2000, §3.5.5). Useful estimators of [**M**] and κ in (8) are the moment estimators, [$\hat{\mathbf{M}}$] and $\hat{\kappa}$, where [$\hat{\mathbf{M}}$] is the sample mean defined in §3.2 and $\hat{\kappa} = (1 - 1/n)^{-1} s^{-2} \langle \bar{\mathbf{t}}, \mathbf{t}([\hat{\mathbf{M}}]) \rangle$ with s^2 the sample variance of $\langle \mathbf{t}([\mathbf{U}]), \mathbf{t}([\hat{\mathbf{M}}]) \rangle$.

Distributions on SO(3)/K can be identified with distributions on SO(3) that are invariant under the action of K. One way of generating such distributions is to average a given distribution on SO(3) over K. This averaging construction has been used by Walsh et al. (2009) in the orthorhombic case, Du et al. (2016) in the cubic case, and by Matthies (1982), Gorelova et al. (2014) and Niezgoda et al. (2016) in the general crystallographic case. Because the parameters of the distributions (5) are readily interpretable and the distributions (6), being exponential models, have pleasant inferential properties, we find these models more useful than many models obtained by averaging over K, especially as the latter can be quite demanding numerically.

5.2 Concentrated distributions

A standard coordinate system on SO(3) is given by the inverse of a restriction of the exponential map $\mathbf{S} \mapsto \sum_{k=0}^{\infty} (k!)^{-1} \mathbf{S}^k$ from the space of skew-symmetric 3×3 matrices to SO(3). This can be modified to provide coordinate systems on SO(3)/K. Let $[\mathbf{M}]$ be an element of SO(3)/K. There are neighbourhoods $\mathcal{N}_{[\mathbf{M}]}$ of $[\mathbf{M}]$ in SO(3)/K and \mathcal{V} of $\mathbf{0}$ in \mathbb{R}^3 such that each $[\mathbf{U}]$ in $\mathcal{N}_{[\mathbf{M}]}$ can be written uniquely as $[\mathbf{U}] = [\mathbf{M} \exp{\{\mathbf{A}(\mathbf{v})\}}]$, where

$$\mathbf{A}(\mathbf{v}) = \begin{pmatrix} o & -v_3 & v_2 \\ v_3 & 0 & -v_1 \\ -v_2 & v_1 & 0 \end{pmatrix}$$

with $\mathbf{v} = (v_1, v_2, v_3)^{\mathrm{T}}$ in \mathcal{V} . Define $p_{[\mathbf{M}]}$ from $\mathcal{N}_{[\mathbf{M}]}$ to \mathcal{V} by $p_{[\mathbf{M}]}([\mathbf{U}]) = \mathbf{v}$, where $[\mathbf{U}] = [\mathbf{M} \exp{\{\mathbf{A}(\mathbf{v})\}}]$. Then $p_{[\mathbf{M}]}$ is a coordinate system on $\mathcal{N}_{[\mathbf{M}]}$. Second-order Taylor expansion about $\mathbf{0}$ of $[\mathbf{U}]$ as a function of \mathbf{v} , together with some computer algebra, gives the high-concentration asymptotic distribution of $[\mathbf{U}]$.

Proposition 2

For [U] near [M] in SO(3)/K put [U] = [M exp {A(v)}] for v near 0 in \mathbb{R}^3 . If [U] has density (6) with $\mathbf{t} = \mathbf{t}_K$ as in Table 2 then the asymptotic distribution of $\kappa^{1/2}\mathbf{v}$ as $\kappa \to \infty$ is normal with mean 0 and variance Σ , where Σ is given in Table 5. If [U] has density (7) with $\mathbf{t} = \mathbf{t}_K$ then $(\kappa/2)^{1/2}\mathbf{v}$ has this asymptotic distribution.

Table 5: High-concentration asymptotic variance, Σ , of $\kappa^{1/2}$.

Group	$oldsymbol{\Sigma}$
C_1	$(1/2)\mathbf{I}_3$
C_2	diag(1/2, 1/4, 1/6)
$C_r (r \ge 3)$	diag $[(1+rA_r)^{-1}, (1+rA_r)^{-1}, \{2rA_r - r(r-1)A_{r-1}\}^{-1}]$
D_2	$(1/4)\mathbf{I}_3$
$D_r (r \ge 3)$	diag $[(rA_r)^{-1}, (rA_r)^{-1}, \{rA_r - r(r-1)A_{r-1}\}^{-1}]$
T	$0.070\mathbf{I}_3$
O	$(1/8)\mathbf{I}_3$
Y	$0.026\mathbf{I}_3$

For C_r and D_r , v_3 is the component of **v** normal to the plane of $\mathbf{u}_1, \dots, \mathbf{u}_r$ and $A_r = \sum_{k=1}^r \cos(k2\pi/r)^r$.

6 Tests of location

6.1 One-sample tests

Let $[\mathbf{M}]$ be an element of SO(3)/K which is some measure of location of a distribution on SO(3)/K. There are various tests of the null hypothesis that $[\mathbf{M}] = [\mathbf{M}_0]$, where $[\mathbf{M}_0]$ is a given element of SO(3)/K. The case with $K = D_2$ was considered by Arnold & Jupp (2013, §8).

Permutation tests can be based on the following symmetries of SO(3)/K: For \mathbf{R} in K, define $\rho_{[\mathbf{M}_0]}(\mathbf{R})$ as the transformation that takes $[\mathbf{U}]$ to $\rho_{[\mathbf{M}_0]}(\mathbf{R})[\mathbf{U}] = [\mathbf{M}_0\mathbf{R}\mathbf{M}_0^{\mathrm{T}}\mathbf{U}]$. Then $\rho_{[\mathbf{M}_0]}(\mathbf{R})$ is well-defined and preserves $[\mathbf{M}_0]$.

For a sample summarized by the sample mean $\bar{\mathbf{t}}$ of \mathbf{t} , an appealing measure of the squared distance between the sample and $[\mathbf{M}_0]$ is $\|\bar{\mathbf{t}} - \mathbf{t}([\mathbf{M}_0])\|^2$. It is appropriate to reject the null hypothesis for large values of $\|\bar{\mathbf{t}} - \mathbf{t}([\mathbf{M}_0])\|^2$. If the distribution of $[\mathbf{U}]$ is symmetric under $\rho_{[\mathbf{M}_0]}$ then significance can be assessed by comparing the observed value of $\|\bar{\mathbf{t}} - \mathbf{t}([\mathbf{M}_0])\|^2$ with its randomization distribution, which can be obtained by replacing $[\mathbf{U}_1], \ldots, [\mathbf{U}_n]$ by $\rho_{[\mathbf{M}_0]}(\mathbf{R}_1)[\mathbf{U}_1], \ldots, \rho_{[\mathbf{M}_0]}(\mathbf{R}_n)[\mathbf{U}_n]$, where $\mathbf{R}_1, \ldots, \mathbf{R}_n$ are independent and distributed uniformly on K.

If $[\mathbf{U}_1], \ldots, [\mathbf{U}_n]$ is a sample from a concentrated distribution with density (6) and mode $[\mathbf{M}]$ then it is sensible to test $H_0 : [\mathbf{M}] = [\mathbf{M}_0]$ by applying Hotelling's 1-sample T^2 test to $p_{[\mathbf{M}_0]}([\mathbf{U}_1]), \ldots, p_{[\mathbf{M}_0]}([\mathbf{U}_n])$, where $p_{[\mathbf{M}_0]}$ is the projection onto the tangent space given in §5.2.

6.2 Two-sample tests

Suppose that two independent random samples $[\mathbf{U}_1], \ldots, [\mathbf{U}_n]$ and $[\mathbf{V}_1], \ldots, [\mathbf{V}_m]$ on SO(3)/K are summarized by the sample means $\bar{\mathbf{t}}_1$ and $\bar{\mathbf{t}}_2$ of $\mathbf{t}([\mathbf{U}_1]), \ldots, \mathbf{t}([\mathbf{U}_n])$ and $\mathbf{t}([\mathbf{V}_1]), \ldots, \mathbf{t}([\mathbf{V}_m])$. Then the squared distance between the two samples can be measured by $\|\bar{\mathbf{t}}_1 - \bar{\mathbf{t}}_2\|^2$. It is appropriate to reject the null hypothesis that the parent populations are the same if $\|\bar{\mathbf{t}}_1 - \bar{\mathbf{t}}_2\|^2$ is large. Significance can be assessed by comparing the observed value of $\|\bar{\mathbf{t}}_1 - \bar{\mathbf{t}}_2\|^2$ with its randomization distribution, obtained by sampling from the potential values corresponding to the partitions of the combined sample into samples of sizes n and m.

Suppose that $[\mathbf{U}_1], \ldots, [\mathbf{U}_n]$ and $[\mathbf{V}_1], \ldots, [\mathbf{V}_m]$ are samples from concentrated distributions with density (6) on SO(3)/K. Let $[\dot{\mathbf{M}}]$ be the maximum likelihood estimate of the mode $[\mathbf{M}]$ under the null hypothesis that the parent populations are the same. Then the null hypothesis can be tested by applying Hotelling's 2-sample T^2 test to $p_{[\dot{\mathbf{M}}]}([\mathbf{U}_1]), \ldots, p_{[\dot{\mathbf{M}}]}([\mathbf{U}_n])$ and

 $p_{[\dot{\mathbf{M}}]}([\mathbf{V}_1]), \dots, p_{[\dot{\mathbf{M}}]}([\mathbf{V}_m])$, where $p_{[\dot{\mathbf{M}}]}$ is the projection onto the tangent space given in §5.2.

7 Independence, regression and misorientation

7.1 Independence

Let $\mathbf{t}_j : SO(3)/K_j \to E$, for j = 1, 2, be equivariant functions into some common inner-product space E such that $\mathbf{t}_j([\mathbf{U}])$ has expectation $\mathbf{0}$ if $[\mathbf{U}]$ is uniformly distributed on $SO(3)/K_j$. Then association of random variables $[\mathbf{U}]$ on $SO(3)/K_1$ and $[\mathbf{V}]$ on $SO(3)/K_2$ can be measured in terms of association of $\mathbf{t}_1([\mathbf{U}])$ and $\mathbf{t}_2([\mathbf{V}])$.

The general approach of Jupp & Spurr (1985) leads to the following test of independence. Given pairs $([\mathbf{U}_1], [\mathbf{V}_1]), \ldots, ([\mathbf{U}_n], [\mathbf{V}_n])$ in $SO(3)/K_1 \times SO(3)/K_2$, independence of \mathbf{U} and \mathbf{V} is rejected for large values of $\sum_{i=1}^n \sum_{j=1}^n \langle \mathbf{t}_1([\mathbf{U}_i]), \mathbf{t}_1([\mathbf{U}_j]) \rangle \langle \mathbf{t}_2([\mathbf{V}_i]), \mathbf{t}_2([\mathbf{V}_j]) \rangle$. The observed value of this statistic is compared with the randomization distribution given $[\mathbf{U}_1], \ldots, [\mathbf{U}_n]$. $[\mathbf{V}_1], \ldots, [\mathbf{V}_n]$. An alternative randomization test rejects independence for large values of the correlation coefficient r defined in (11). For $K_1 = K_2 = C_1$ and $\mathbf{t}_1 = \mathbf{t}_2 = \mathbf{t}_{C_1}$ of Table 2, this is one of the tests considered by Rivest & Chang (2006).

7.2 Regression

A reasonable model for homoscedastic regression of [V] in $SO(3)/K_2$ on [U] in $SO(3)/K_1$ has regression function [U] \mapsto [AU] for some A in SO(3) and error distribution that is a mild generalization of (6), so that the density of [V] given [U] is

$$f([\mathbf{V}] \mid [\mathbf{U}]; \mathbf{A}, \kappa) = c(\kappa)^{-1} \exp\{\kappa \langle \mathbf{t}_2([\mathbf{V}]), \mathbf{t}_1([\mathbf{A}\mathbf{U}]) \rangle\}.$$
 (9)

For $K_1 = K_2 = C_1$ and $\mathbf{t}_1 = \mathbf{t}_2 = \mathbf{t}_{C_1}$ of Table 2 , model (9) is a generalization of the spherical regression model of Chang (1986). It is the submodel $\mathbf{A}_2 = \mathbf{I}_3$ of the models with regression function $\mathbf{U} \mapsto \mathbf{A}\mathbf{U}\mathbf{A}_2$ that were introduced by Prentice (1989) and explored by Chang & Rivest (2001) and Rivest & Chang (2006). For $K_1 \neq C_1$, it is not possible in general to extend the model (9) to have regression function of the form $[\mathbf{U}] \mapsto [\mathbf{A}\mathbf{U}\mathbf{A}_2]$. If $K_1 \neq K_2$ then the \mathbf{t}_j given in Table 3.1 are not suitable, since in many cases $\langle \mathbf{t}_2([\mathbf{V}]), \mathbf{t}_1([\mathbf{A}\mathbf{U}]) \rangle = 0$ for all values of $[\mathbf{U}]$, $[\mathbf{V}]$ and \mathbf{A} . Instead, it is sensible to take $E = L^2(SO(3))$ and the \mathbf{t}_j obtained by the averaging construction described in the first paragraph of §3.1.

For $\kappa > 0$, the maximum likelihood estimate of **A** is

$$\hat{\mathbf{A}} = \arg \max_{\mathbf{A} \in SO(3)} \sum_{i=1}^{n} \langle \mathbf{t}_2([\mathbf{V}_i]), \mathbf{t}_1([\mathbf{A}\mathbf{U}_i]) \rangle.$$
 (10)

In general, $\hat{\mathbf{A}}$ is a well-defined element of SO(3), rather than an element of some quotient.

Put $\rho_{12} = \max_{\mathbf{U} \in SO(3)} \langle \mathbf{t}_1([\mathbf{U}]), \mathbf{t}_2([\mathbf{I}_3]) \rangle$. If $\rho_{12} > 0$ then define

$$r = (n\rho_{12})^{-1} \sum_{i=1}^{n} \langle \mathbf{t}_1([\hat{\mathbf{A}}\mathbf{U}_i]), \mathbf{t}_2([\mathbf{V}_i]) \rangle, \tag{11}$$

where $\hat{\mathbf{A}}$ is given by (10). Then $-1 \leq r \leq 1$ and r can be regarded as a form of uncorrected sample correlation of $[\mathbf{U}]$ and $[\mathbf{V}]$. If $K_1 = K_2 = D_2$, n = 1 and $\mathbf{t}_1 = \mathbf{t}_2 = \mathbf{t}$ is defined by $\mathbf{t}([\mathbf{U}]) = \mathbf{U}\operatorname{diag}(1,0,-1)\mathbf{U}^{\mathrm{T}}$ then $r = \cos \omega$, where ω is the misorientation angle for D_2 introduced by Tape & Tape (2012). Application of Proposition 2 to the decomposition

$$\begin{split} &\sum_{i=1}^{n} \left\{ \rho^{2} - \langle \mathbf{t}([\mathbf{I}_{3}]), \mathbf{t}([\mathbf{V}_{i}^{\mathrm{T}}\mathbf{A}\mathbf{U}_{i}]) \rangle \right\} \\ &= \sum_{i=1}^{n} \left\{ \rho^{2} - \langle \mathbf{t}([\mathbf{I}_{3}]), \mathbf{t}([\mathbf{V}_{i}^{\mathrm{T}}\hat{\mathbf{A}}\mathbf{U}_{i}]) \rangle \right\} \\ &+ \sum_{i=1}^{n} \left\{ \langle \mathbf{t}([\mathbf{I}_{3}]), \mathbf{t}([\mathbf{V}_{i}^{\mathrm{T}}\hat{\mathbf{A}}\mathbf{U}_{i}]) \rangle - \langle \mathbf{t}([\mathbf{I}_{3}]), \mathbf{t}([\mathbf{V}_{i}^{\mathrm{T}}\mathbf{A}\mathbf{U}_{i}]) \rangle \right\} \end{split}$$

gives the following high-concentration asymptotic distributions.

Proposition 3

For
$$(\mathbf{U}_1, \mathbf{V}_1), \dots, (\mathbf{U}_n, \mathbf{V}_n)$$
 from model (9),

(i) Asymptotically, for large κ ,

$$2\kappa \sum_{i=1}^{n} \left\{ \rho^{2} - \langle \mathbf{t}([\mathbf{I}_{3}]), \mathbf{t}([\mathbf{V}_{i}^{\mathrm{T}}\mathbf{A}\mathbf{U}_{i}]) \rangle \right\} \sim \chi_{3n}^{2},$$

$$2\kappa \sum_{i=1}^{n} \left\{ \rho^{2} - \langle \mathbf{t}([\mathbf{I}_{3}]), \mathbf{t}([\mathbf{V}_{i}^{\mathrm{T}}\hat{\mathbf{A}}\mathbf{U}_{i}]) \rangle \right\} \sim \chi_{3(n-1)}^{2}, (12)$$

$$2\kappa \sum_{i=1}^{n} \left\{ \langle \mathbf{t}([\mathbf{I}_{3}]), \mathbf{t}([\mathbf{V}_{i}^{\mathrm{T}}\hat{\mathbf{A}}\mathbf{U}_{i}]) \rangle - \langle \mathbf{t}([\mathbf{I}_{3}]), \mathbf{t}([\mathbf{V}_{i}^{\mathrm{T}}\mathbf{A}\mathbf{U}_{i}]) \rangle \right\} \sim \chi_{3}^{2}. (13)$$

and the quantities in (12) and (13) are asymptotically independent.

(ii) An approximate high-concentration $100(1-\alpha)\%$ confidence region for **A** is

$$\left\{\mathbf{A}: 2\hat{\kappa} \sum_{i=1}^{n} \left\{ \langle \mathbf{t}([\mathbf{I}_{3}]), \mathbf{t}([\mathbf{V}_{i}^{\mathrm{T}} \hat{\mathbf{A}} \mathbf{U}_{i}]) \rangle - \langle \mathbf{t}([\mathbf{I}_{3}]), \mathbf{t}([\mathbf{V}_{i}^{\mathrm{T}} \mathbf{A} \mathbf{U}_{i}]) \rangle \right. \right. \right\} < \chi_{3;\alpha}^{2} \right\}.$$

7.3 Misorientation

The relationship between ambiguous rotations [U] in $SO(3)/K_1$ and [V] in $SO(3)/K_2$ can be described by the misorientation, which is an element of the double coset space $K_1 \setminus SO(3)/K_2$. Since [U] and [V] are images of UR₁ and VR_2 in SO(3) for any R_1 in K_1 and R_2 in K_2 , $(UR_1)^T VR_2$ determines a well-defined element of $K_1 \setminus SO(3)/K_2$. See p. 274 of Morawiec (1997). In crystallography it is usual to identify $K_1 \setminus SO(3)/K_2$ with an asymmetric domain, a neighbourhood of $\mathbf{0}$ in \mathbb{R}^3 that is in one-to-one correspondence, modulo null sets, with $K_1 \setminus SO(3)/K_2$ under $\mathbf{v} \mapsto \exp\{\mathbf{A}(\mathbf{v})\}$ followed by projection of SO(3) to $K_1 \setminus SO(3) / K_2$. Then the misorientation between [U] and [V] is taken as the element, P, of the asymmetric domain that satisfies $\mathbf{V} = \mathbf{UP}$ and has smallest rotation angle among all such rotations in the domain. In the case in which the conditional distribution of [V] given [U] is uniform the distributions of the angle and axis of the misorientation are given in Morawiec (2004, Ch. 7). For general pairs $([\mathbf{U}_1], [\mathbf{V}_1]), \dots, ([\mathbf{U}_n], [\mathbf{V}_n])$ in $SO(3)/K_1 \times SO(3)/K_2$, we define the mean misorientation as the element A of SO(3) defined in (10). An alternative definition of the mean misorientation is the element $(\hat{\mathbf{A}}_1, [\hat{\mathbf{A}}_2])$ of $SO(3) \times (K \setminus SO(3))$ that maximizes $\sum_{i} \max_{\mathbf{R}_i \in K} \langle \mathbf{t}_1([\mathbf{A}_1 \mathbf{U}_i]), \mathbf{t}_2([\mathbf{V}_i \mathbf{R}_i \mathbf{A}_2]) \rangle.$

8 Example

To illustrate the estimators and tests introduced above, we consider some samples of orientations of diopside crystals. These crystals are monoclinic, so we can represent their orientations by C_2 -frames.

The stereonet in Fig. 1 shows the \mathbf{u}_0 vectors and $\pm \mathbf{u}_1$ axes given by orientations of 100 diopside crystals. A randomization test of uniformity based on S from (3) in §4.1 has p-value less than 0.001, leading to decisive rejection of uniformity.

The stereonets in Fig. 2 show the \mathbf{u}_0 vectors and $\pm \mathbf{u}_1$ axes given by orientations of 34 crystals from one region of a specimen and 37 crystals

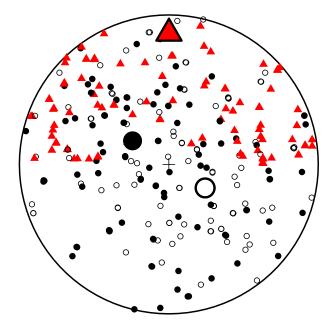


Figure 1: Stereonet of \mathbf{u}_0 vectors, shown as red triangles, and $\pm \mathbf{u}_1$ axes, shown as circles, given by orientations of 100 diopside crystals. The disc is a stereographic projection of these vectors and axes, showing the whole of the sphere, so that each axis appears twice with filled circles denoting the lower ends of axes and open circles the upper ends. The sample mean is shown in large symbols.

from another region. The two-sample permutation test of $\S6.2$ yields a p-value of 0.07 for equality of the populations of the orientations in the two regions, so the hypothesis of equality is not rejected.

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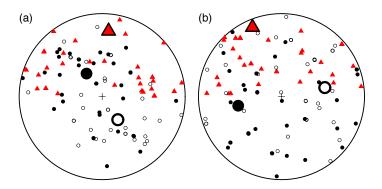


Figure 2: Stereonets of \mathbf{u}_0 vectors, shown as red triangles, and $\pm \mathbf{u}_1$ axes, shown as circles, given by orientations of two samples of diopside crystals. Each disc is a stereographic projection of these axes and vectors, showing the whole of the sphere, so that each axis appears twice. (a): 34 orientations from one region of a specimen. (b): 37 orientations from another region. The sample means are shown as large symbols.

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