SECOND PAPER ON STATISTICS ASSOCIATED WITH THE RANDOM DISORIENTATION OF CUBES

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Theoretical density functions are obtained for the angle of disorientation (the least angle of rotation required to rotate a cube into a standard orientation) and for Min⟨100⟩ (the least of the nine acute angles between the edges of a cube and the edges of a fixed reference cube). These density functions and their cumulative distribution functions have been evaluated numerically.

1. Introduction

In a recent paper Mackenzie & Thomson (1957) described a class of problems in three-dimensional geometrical probability, and some of the associated density functions were estimated numerically by means of random sampling. In this paper two of these density functions are obtained in analytical form and, together with their cumulative distribution functions, evaluated numerically.†

The two density functions obtained are those for the angle of disorientation and Min ⟨100⟩. These two variables can be defined as follows. Consider two cubes, A and B, and imagine A to be a reference cube with its edges parallel to a fixed set of co-ordinate axes and its centre at the origin, while B is initially coincident with A but free to rotate in any manner about the common centre of A and B. If B is given an arbitrary rotation there are 24 definite rotations which will restore B into coincidence with A; these are just the reverse of the original rotation taken together with the 24 proper symmetry operations associated with a cube having indistinguishable faces (see § 2). The angle of disorientation is the least (in magnitude) of the 24 angles of rotation so obtained, while Min ⟨100⟩ is the least of the nine acute angles between the edges of the cube B in an arbitrary orientation and the edges of A.

The success of the present calculations has depended essentially on reducing the amount of detailed calculation required although this is still quite considerable. Since this reduction can be made for a whole class of problems, including the two special cases discussed in detail, a formulation of this class is given in § 2 together with their formal solution in a form which is of no practical use. Section 3 is devoted to reductions common to the whole class, while § 4 completes the reduction for the two special cases. The fact that these reductions involve arguments which are basically of a group-theoretical nature suggests that a more systematic use of group theory might make practicable a solution for the whole class.

The density functions for the angle of disorientation and Min ⟨100⟩ are given both analytically and numerically in §§ 5 and 6. A large amount of algebraic detail has been omitted in these sections and only a few important intermediate results are given.

† Following the preparation of the paper by Miss Thomson and myself, a copy of which was sent via Mr Hammersley to Mr D. C. Handscomb, the latter wrote to me to say that he had found the exact distributions of the angle of disorientation by geometrical means, and gave the formulae (5·3), (5·5) and (5·6) of my paper below. His method (the particulars of which I have not seen at the time of writing) is, I understand, quite different from mine and I have therefore given my own derivation in full. His paper, I am informed, is to appear in the Canadian Journal of Mathematics.

2. Formulation of problems

Since the group of symmetry operations on a cube with indistinguishable faces (the cubic group) plays a fundamental role in both the formulation and the reduction of the class of problems, a brief statement of these symmetry operations will first be given.

If the cube A has indistinguishable faces it is invariant under the 48 symmetry operations of the cubic group consisting of 24 proper rotations and 24 improper rotations, which are proper rotations together with an inversion or a reflexion. The 24 proper rotations are (*a*) the identity element or no rotation, (*b*) rotations of $180°$ about the three axes of reference, (*c*) rotations of $\pm 90°$ about the same axes, (*d*) rotations of $180°$ about axes parallel to the six face diagonals of the cube, and (*e*) rotations of $\pm 120°$ about axes parallel to the four diagonals of the cube. On taking axes of reference parallel to the edges of the cube these 24 rotations can be represented by 3×3 orthogonal matrices. These matrices have only three non-zero elements which are either $+1$ or -1 and these are arranged in all possible ways such that there is a non-zero element in each row and column and the determinant of the matrix is $+1$.

In all that follows, the matrices representing these proper symmetry rotations will be denoted by $\mathbf{S}_i$ $(i = 1, \ldots, 24)$; the improper rotations are then $-\mathbf{S}_i$. Further, the 3×3 orthogonal matrix which represents an arbitrary proper rotation through an angle ψ about an axis in the direction $\mathbf{n} = [n_1 n_2 n_3]$ will be denoted by $\mathbf{R}$ with elements r_{ij} given by (3·1) and this rotation will be described briefly as either the rotation $\mathbf{R}$, the rotation $\psi, \mathbf{n}$ or the rotation $\psi[n_1 n_2 n_3]$.

Since
$$\operatorname{Tr}(\mathbf{R}) = r_{11}+r_{22}+r_{33} = 1+2\cos\psi, \tag{2·1}$$
it follows that the angle of disorientation ψ_d is given by
$$\begin{aligned} 1+2\cos\psi_d &= \operatorname*{Max}_{j} \operatorname{Tr}(\mathbf{R}\mathbf{S}_j), \\ &= \operatorname*{Max}_{i,j} \operatorname{Tr}(\mathbf{S}_i\mathbf{R}\mathbf{S}_j), \end{aligned} \tag{2·2}$$
on using the facts that for any matrices $\mathbf{B}, \mathbf{C}$ $\operatorname{Tr}(\mathbf{BC}) = \operatorname{Tr}(\mathbf{CB})$ provided both products exist and that the product $\mathbf{S}_j\mathbf{S}_i$ is another symmetry rotation.

Further, a generalized variable Min $\langle uvw\rangle$ can be defined as follows. Let $\mathbf{u}$ be a 3×1 column matrix with elements equal to the direction cosines of the direction $[uvw]$, so that the set $\langle uvw\rangle$ of variants of $[uvw]$ are the 24 directions $\mathbf{S}_i\mathbf{u}$ together with the 24 directions $-\mathbf{S}_i\mathbf{u}$. Thus, the cosine of the angle θ_{ij} between a variant, $\pm\mathbf{S}_i\mathbf{u}$, and what another variant, $\pm\mathbf{S}_j\mathbf{u}$, becomes after a rotation $\mathbf{R}$, is given by $\cos\theta_{ij} = \pm\mathbf{u}'\mathbf{S}_i'\mathbf{R}\mathbf{S}_j\mathbf{u}$ when the usual scalar product is written in matrix notation. Then
$$\cos(\operatorname{Min}\langle uvw\rangle) = \operatorname*{Max}_{i,j} |\,\mathbf{u}'\mathbf{S}_i\mathbf{R}\mathbf{S}_j\mathbf{u}\,|, \tag{2·3}$$
$$= \operatorname*{Max}_{i,j} |\operatorname{Tr}(\mathbf{S}_i\mathbf{R}\mathbf{S}_j\mathbf{u}\mathbf{u}')|. \tag{2·4}$$

Since the variants $\langle 100\rangle$ of $[100]$ are parallel to the edges of the cube A the definition of Min $\langle 100\rangle$ given in the introduction is a special case of (2·3). Equation (2·4) leads to an equivalent definition of Min $\langle 100\rangle$. For, if $\mathbf{u} = [100]$, $\mathbf{S}_j\mathbf{u}\mathbf{u}'\mathbf{S}_i$ is a matrix with only one non-zero element which is ± 1 and may be in any position in the matrix; the trace of the product with $\mathbf{R}$ then gives $\pm$ the corresponding element in $\mathbf{R}'$. Thus, the cosine of the angle Min $\langle 100\rangle$ is the largest of the moduli of the elements of the orthogonal 3×3 matrix $\mathbf{R}$.

If in (2·4) the $\mathbf{S}_i$, $\mathbf{S}_j$ are allowed to range over the full cubic group, the modulus sign can be dropped. Then comparison of (2·2) with (2·4) shows that all cases are special cases of

$$x(\mathbf{A}) = \operatorname*{Max}_{i,j} \mathrm{Tr}\,(\mathbf{S}_i \mathbf{R} \mathbf{S}_j \mathbf{A}), \tag{2·5}$$

where $\mathbf{A}$ is a given (symmetric) matrix and the $\mathbf{S}$ range independently either over the whole cubic group or over the subgroup of proper rotations. If $V(\mathbf{R})$ is a given probability measure on the space of (proper) orthogonal matrices, the cumulative distribution function of $x(\mathbf{A})$ is

$$P\{x(\mathbf{A}) < X\} = \int dV(\mathbf{R}), \tag{2·6}$$

where the region of integration includes all $\mathbf{R}$ for which

$$x(\mathbf{A}) < X. \tag{2·7}$$

This formal solution is no more than a statement of what is required and the practical problem is first to assign a suitable measure to $V(\mathbf{R})$ and second to determine the region of integration.

3. THE PROBABILITY MEASURE AND REDUCTION OF THE REGION OF INTEGRATION

When concerned with problems in geometrical probability the appropriate probability measure is determined by a principle of invariance enunciated by Deltheil (1926, p. 13). This principle asserts that the result of the calculation must be invariant for any displacement of the whole figure. In the present case, this means invariant for any rotation of the cubes A and B together as a unit.

Writing $c = 1-\cos\psi$ and $s = \sin\psi$, the rotation ψ, $\mathbf{n}$ has the matrix representation

$$\mathbf{R} = \begin{pmatrix} 1-c+n_1^2c, & n_1n_2c-n_3s, & n_1n_3c+n_2s \\ n_1n_2c+n_3s, & 1-c+n_2^2c, & n_2n_3c-n_1s \\ n_1n_3c-n_2s, & n_2n_3c+n_1s, & 1-c+n_3^2c \end{pmatrix}, \tag{3·1}$$

and in this case Deltheil (1926, p. 105) shows that the element of probability measure is given by

$$dV(\mathbf{R}) = (1/2\pi^2)\sin^2\tfrac{1}{2}\psi\, d\psi\, dS, \tag{3·2}$$

where dS is an element of area on the surface of the unit (hemi-) sphere $n_1^2+n_2^2+n_3^2 = 1$ and, if spherical polar co-ordinates θ, ϕ are used to specify the axis of rotation

$$dS = \sin\theta\, d\theta\, d\phi. \tag{3·3}$$

The whole space of $\mathbf{R}$ is covered once if $-\pi \leqslant \psi \leqslant \pi$, $0 \leqslant \phi \leqslant 2\pi$ and $0 \leqslant \theta \leqslant \frac{1}{2}\pi$, and the total volume of the space is unity.

The density function defined by (3·2) is the analogue of a uniform density for a one-dimensional variable with a finite range. Further, the invariance properties of this density and its uniqueness arising therefrom ensure that it is identical with that implied by Mackenzie & Thomson (1957) in the construction of their random orthogonal matrices.

The region of integration can now be subdivided into $24^2 = 576$ equivalent regions. For, consider the pair of rotations $\mathbf{R}$ and $\mathbf{S}_k\mathbf{R}\mathbf{S}_l$. Since products of the type $\mathbf{S}_i\mathbf{S}_k$ or $\mathbf{S}_l\mathbf{S}_j$ run through the complete sequence of symmetry rotations as $\mathbf{S}_i$ or $\mathbf{S}_j$ do so, it follows from (2·5) that the value of $x(\mathbf{A})$ is the same for both rotations. But the invariance properties of the probability measure defined by (3·2) ensure that corresponding regions in the neighbourhood of the two rotations have equal volumes and so only 1/576 of the total volume need be considered.

The same result can also be reached using the geometrical model mentioned in the introduction. For suppose that the cube B is subjected to the sequence of rotations $\mathbf{S}_k\mathbf{R}\mathbf{S}_l$. The above result now follows on using Deltheil's principle of invariance, provided that the final geometrical relationship between the cubes A and B is the same whatever the symmetry rotations $\mathbf{S}_k$, $\mathbf{S}_l$ may be. That this is so can be seen as follows. After the symmetry rotation $\mathbf{S}_l$ the cube B is still coincident with the cube A so that after the further rotation $\mathbf{R}$ the relationship between A and B is independent of $\mathbf{S}_l$. If the two cubes are now rotated together as a rigid body by the rotation $\mathbf{S}_k$, the cube B reaches its final orientation and A remains invariant; thus, the final relationship between the cubes A and B is independent of $\mathbf{S}_k$ also.

Although a preliminary subdivision of the region of integration into 24 equivalent regions can be defined in a simple way in the general case, the further subdivision of each of these regions into 24 parts is carried out in a manner suited to the two special problems. The preliminary subdivision is determined by the fact that if $\mathbf{R}$ represents a rotation $\psi, \mathbf{n}$ then $\mathbf{SRS}^{-1}$ represents a rotation $\psi, \mathbf{Sn}$. The end-point of the unit vector $\mathbf{n}$ lies on the surface of a unit hemisphere and the product $\mathbf{Sn}$ simply permutes the components of $\mathbf{n}$ in order and sign. Thus, the surface of the unit hemisphere can be divided into 24 equivalent spherical triangles bounded by great circles for which either the moduli of two components of $\mathbf{n}$ are equal or one of the components is zero. It suffices to consider those axes $\mathbf{n}$ which lie in any one of these triangles.

Since rotations about the same axis and through the same angle but in opposite senses leaves the geometrical relationship between the cubes A and B unchanged, a further halving of the region of integration is achieved. Thus, it may be assumed that the angle of rotation ψ is positive and that the axis of rotation lies in the spherical triangle defined by

$$n_1 \geqslant n_2 \geqslant n_3 \geqslant 0.$$

4. The region of integration

It is convenient to carry out first the final subdivision and specification of the region of integration for the case of the angle of disorientation and then show that the same region is suitable for Min $\langle 100 \rangle$.

Given any rotation $\mathbf{R}$ there is, in general, just one equivalent rotation $\mathbf{RS}_1$ for which the angle of rotation is minimum.† Then, there is a unique equivalent matrix $\mathbf{R}^* = \mathbf{S}_2\mathbf{RS}_1\mathbf{S}_2^{-1}$ for which the angle of rotation is least and the axis of rotation lies in the triangle defined by $n_1 \geqslant n_2 \geqslant n_3 \geqslant 0$. But according to the result obtained in the last section it suffices to consider only those rotations $\mathbf{R}$ for which $\psi \geqslant 0$ and $n_1 \geqslant n_2 \geqslant n_3 \geqslant 0$. The final reduction of the region of integration is now determined by the conditions which ensure that $\mathbf{R} = \mathbf{R}^*$.

When $\mathbf{R}$ is given by (3·1), calculation shows that the cosine of half the angle of rotation determined by the matrix $\mathbf{RS}$ is given by the modulus of one of the five expressions

$$\left.\begin{array}{ll} \cos\frac{1}{2}\psi, & n_1 \sin\frac{1}{2}\psi, \\ (n_1 \sin\frac{1}{2}\psi + \cos\frac{1}{2}\psi)/\sqrt{2}, & [(n_1+n_2)\sin\frac{1}{2}\psi]/\sqrt{2}, \\ \frac{1}{2}(n_1+n_2+n_3)\sin\frac{1}{2}\psi + \frac{1}{2}\cos\frac{1}{2}\psi, & \end{array}\right\} \qquad (4·1)$$

† If this angle happens to be negative the transposed (or inverse) matrix represents an equivalent rotation through a positive angle.

together with the modulus of what these five expressions become when n_1, n_2, n_3 are permuted in all possible ways in order and in sign (24 values in all). Those written down correspond to the cases where $\mathbf{S}$ is the rotation identity, $180°[100]$, $90°[100]$, $180°[110]$ and $-120°[111]$. Clearly, when $0 \leqslant \psi \leqslant \pi$ and $n_1 \geqslant n_2 \geqslant n_3 \geqslant 0$, the largest value of the cosine will be one of those set out explicitly in (4·1).

If $\mathbf{R} = \mathbf{R}^*$, then $\cos \frac{1}{2}\psi$ must be the greatest of the five expressions in (4·1) and after some manipulation of inequalities the region of integration is found to be

$$\left.\begin{aligned} &0 \leqslant \tan \tfrac{1}{2}\psi \leqslant (\sqrt{2}-1)/n_1 && \text{for} \quad \sqrt{2}\,n_1 \geqslant n_2+n_3, \\ &0 \leqslant \tan \tfrac{1}{2}\psi \leqslant 1/(n_1+n_2+n_3) && \text{for} \quad \sqrt{2}\,n_1 \leqslant n_2+n_3, \\ &n_1 \geqslant n_2 \geqslant n_3 \geqslant 0. \end{aligned}\right\} \tag{4·2}$$

The same region is also suitable for Min $\langle 100 \rangle$ since r_{11} is the greatest element in $\mathbf{R}^*$. For, within the region (4·2), it is easily shown by using (3·1) that

$$\left.\begin{aligned} &r_{11} \geqslant r_{22} \geqslant r_{33} \geqslant 0, \\ &r_{32} \geqslant r_{13} \geqslant r_{21} \geqslant r_{12} \geqslant r_{31} \geqslant r_{23}, \end{aligned}\right\} \tag{4·3}$$

and that $r_{21} \geqslant 0$, $r_{31} \leqslant 0$, while r_{12} may be either positive or negative. Finally $r_{11} \geqslant r_{32}$ provided

$$[1-(n_1+n_2+n_3)\tan \tfrac{1}{2}\psi]\,[1-(n_1-n_2-n_3)\tan \tfrac{1}{2}\psi] \geqslant 0, \tag{4·4}$$

and in the region (4·2) both factors are positive.

5. The angle of disorientation

When attention is restricted to the region of integration defined by (4·2) and the axis of rotation is specified in spherical polar co-ordinates the probability element (3·2) becomes

$$dV(\mathbf{R}^*) = (576/\pi^2) \sin\theta \sin^2 \tfrac{1}{2}\psi \, d\theta \, d\phi \, d\psi. \tag{5·1}$$

Thus, the density function for the angle of disorientation ψ is found by integrating (5·1) with respect to θ and ϕ with ψ fixed and for all θ and ϕ within the region (4·2), i.e. over part of a unit sphere.

The spherical triangle within which $n_1 \geqslant n_2 \geqslant n_3 \geqslant 0$ is shown as STU on part of a stereographic projection (Barrett, 1952) in Fig. 1. The region $ABSU$ contains that part of the region of integration determined by the first set of inequalities in (4·2) while ABT contains the part determined by the second set. Now for a fixed ψ the first inequality of (4·2) can be written

$$n_1 \leqslant (\sqrt{2}-1)/\tan \tfrac{1}{2}\psi, \tag{5·2}$$

and it is clear that for $0 \leqslant \tan \frac{1}{2}\psi \leqslant \sqrt{2}-1$ or $0 \leqslant \psi \leqslant 45°$, this is always satisfied. Similarly, the second inequality is always satisfied for $0 \leqslant \psi \leqslant 60°$. Thus, for $0 \leqslant \psi \leqslant 45°$ the region of integration is the whole of STU. When $\psi > 45°$, equality in (5·2) determines a small circle P_0Q_0 with its centre at [100], so that for $45° \leqslant \psi \leqslant 60°$ the region of integration is STU with the part SP_0Q_0 removed. Likewise when ψ is just greater than 60° a part $TP_1'Q_1'$ determined by a small circle centred on [111] is removed from consideration so that only the region $P_1P_1'Q_1'UQ_1$ remains; it is readily verified that the arc P_1Q_1 is just short of a small circle joining U and B. As ψ increases further the arcs P_1Q_1 and $P_1'Q_1'$ move towards one another until P_1 and P_1' coincide with B (and Q_1 with U) when $\tan \frac{1}{2}\psi = \sqrt{2}\,(\sqrt{2}-1)$ or $\psi = 60{\cdot}72°$. Finally, the common point P_2 moves along the arc BA until the region of integration $P_2Q_2Q_2'$ disappears at A when $\tan \frac{1}{2}\psi = (\sqrt{2}-1)\,(5-2\sqrt{2})^{\frac{1}{2}}$ or $\psi = 62{\cdot}80°$.

Thus, there are four ranges of ψ to consider and, within each, the density function takes a different analytical form. Each range is considered in turn below and the densities have all been multiplied by $\frac{1}{180}\pi$ so that ψ is measured in degrees.

(*a*) $0 \leqslant \tan\frac{1}{2}\psi \leqslant \sqrt{2}-1$ or $0 \leqslant \psi \leqslant 45^\circ$. The surface area of the triangle STU is $\frac{1}{12}\pi$ so that the density function is

$$p(\psi) = (2/15)(1-\cos\psi). \tag{5·3}$$

(*b*) $\sqrt{2}-1 \leqslant \tan\frac{1}{2}\psi \leqslant 1/\sqrt{3}$ or $45^\circ \leqslant \psi \leqslant 60^\circ$. In this case, a contribution from the area SP_0Q_0 must be subtracted from (5·3). Using polar co-ordinates θ, ϕ with [100] as pole and $\phi = 0$ on SU the area SP_0Q_0 is given by

$$\tfrac{1}{4}\pi\int_{n_1}^{1} dx = \tfrac{1}{4}\pi[1-(\sqrt{2}-1)\cot\tfrac{1}{2}\psi], \tag{5·4}$$

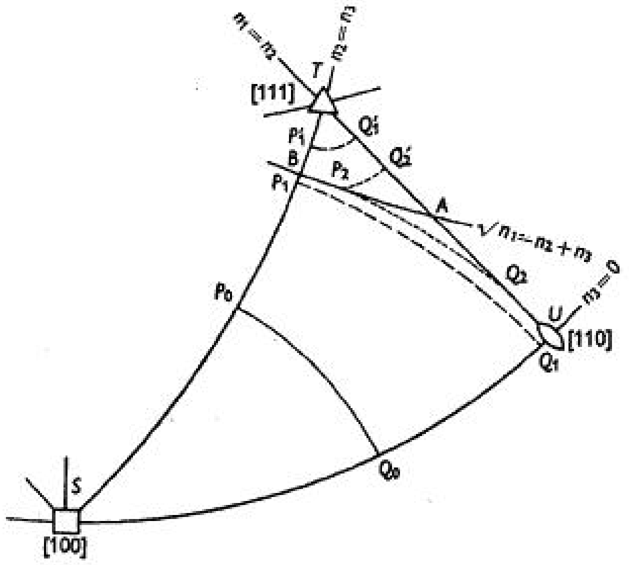

Fig. 1. Part of a stereographic projection of a hemisphere, showing the region of integration for calculating the density function for the angle of disorientation.

where $x = \cos\theta$ and n_1 is given by (5·2) with the sign of equality. Thus,

$$p(\psi) = (2/15)[3(\sqrt{2}-1)\sin\psi - 2(1-\cos\psi)]. \tag{5·5}$$

(*c*) $1/\sqrt{3} \leqslant \tan\frac{1}{2}\psi \leqslant \sqrt{2}(\sqrt{2}-1)$ or $60^\circ \leqslant \psi \leqslant 60{\cdot}72^\circ$. In addition to the area given by (5·4) the area of the region $TP_1'Q_1'$ must also be subtracted from STU. This is most simply done in terms of polar co-ordinates with [111] as pole and $\phi = 0$ on ST; the range of ϕ is to $\frac{1}{3}\pi$ and the limits for $\cos\theta$ are 1 and $(\cot\frac{1}{2}\psi)/\sqrt{3}$. The final result is

$$p(\psi) = (2/15)[\{3(\sqrt{2}-1)+4/\sqrt{3}\}\sin\psi - 6(1-\cos\psi)]. \tag{5·6}$$

(*d*) $\sqrt{2}(\sqrt{2}-1) \leqslant \tan\frac{1}{2}\psi \leqslant (\sqrt{2}-1)(5-2\sqrt{2})^{\frac{1}{2}}$ or $60{\cdot}72^\circ \leqslant \psi \leqslant 62{\cdot}80^\circ$. This case is a little more complicated than the preceding cases as it involves finding the area of the region BP_2Q_2U (where B and U are joined by a small circle centred at [100]) and the area of an analogous region on the other side of AB. Using polar co-ordinates as in (*b*), it is found that for a fixed θ the extreme values of ϕ at points such as Q_2 and P_2 are arcos (cot θ) and $\frac{1}{4}\pi$ – arcos (cot θ) respectively. Thus the area of BP_2Q_2U is given by

$$\int_{n_1}^{1/\sqrt{2}} [\tfrac{1}{4}\pi - 2\,\mathrm{arcos}\,\{x/(1-x^2)^{\frac{1}{2}}\}]\,dx, \tag{5·7}$$

where x and n_1 are the same as in (b). Similarly, using [111] as pole as in (c) the analogous area on the other side of AB is found to be

$$\int [\tfrac{1}{3}\pi - \mathrm{arcos}\,\{(\sqrt{2}-1)^2\,x/(1-x^2)^{\frac{1}{2}}\}]\,dx, \tag{5·8}$$

the range of integration being from $(\cot\frac{1}{2}\psi)/\sqrt{3}$ to $(\sqrt{2}+1)/\sqrt{6}$. Finally, evaluating all the integrals and combining the results as required gives

$$\begin{aligned} p(\psi) = {} & (2/15)\,[\{3(\sqrt{2}-1)+4/\sqrt{3}\}\sin\psi - 6(1-\cos\psi)] \\ & -(8/5\pi)\,[2(\sqrt{2}-1)\,\mathrm{arcos}\,(X\cot\tfrac{1}{2}\psi)+(1/\sqrt{3})\,\mathrm{arcos}\,(Y\cot\tfrac{1}{2}\psi)]\sin\psi \\ & +(8/5\pi)\,[2\,\mathrm{arcos}\,\{(\sqrt{2}+1)\,X/\sqrt{2}\}+\mathrm{arcos}\,\{(\sqrt{2}+1)\,Y/\sqrt{2}\}]\,(1-\cos\psi), \end{aligned} \tag{5·9}$$

where

$$\left.\begin{aligned} X &= (\sqrt{2}-1)/[1-(\sqrt{2}-1)^2\cot^2\tfrac{1}{2}\psi]^{\frac{1}{2}}, \\ Y &= (\sqrt{2}-1)^2/[3-\cot^2\tfrac{1}{2}\psi]^{\frac{1}{2}}. \end{aligned}\right\} \tag{5·10}$$

The density function has been computed from (5·3), (5·5), (5·6) and (5·9) and is tabulated together with the cumulative distribution function in Table 1; the latter function was obtained by numerical integration of the density function. The mean, the standard deviation and the median were calculated to be

$$\bar{\psi} = 40{\cdot}736^\circ, \quad \sigma = 11{\cdot}315^\circ, \quad \psi_{\text{med.}} = 42{\cdot}341^\circ. \tag{5·11}$$

Table 1. *Distribution of the angle of disorientation*

ψ°	$p(\psi)$	C.D.F.†	ψ°	$p(\psi)$	C.D.F.†
0	0·00000	0·00000	60·0	0·01015	0·99228
5	·00051	·00085	60·2	·00856	·99415
10	·00203	·00676	60·4	·00695	·99570
15	·00454	·02277	60·6	·00533	·99693
20	·00804	·05383	60·72...	·00434	·99752
25	0·01249	0·10477	61·0	0·00283	0·99850
30	·01786	·18028	61·4	·00151	·99935
35	·02411	·28487	61·8	·00070	·99978
40	·03119	·42280	62·2	·00024	·99996
45	·03905	·59810	62·6	·00003	1·00000
50	0·03167	0·77586	62·799...	0·00000	1·00000
55	·02201	·91097			
60	·01015	·99228			

† C.D.F. = cumulative distribution function.

The density function has also been plotted in Fig. 2 and has a sharp peak at 45°; in fact the first derivative is discontinuous at $\psi = 45$ and $60°$, while the second derivative is discontinuous at 60·72°. This confirms substantially the guess made by Mackenzie & Thomson (1957) concerning the true nature of the distribution. The dots on Fig. 2 give a graphically smoothed estimate of the density function obtained from the random sampling calculations. The agreement between this estimate and the true density function is rather better than that expected since a sample of only 150 was used.

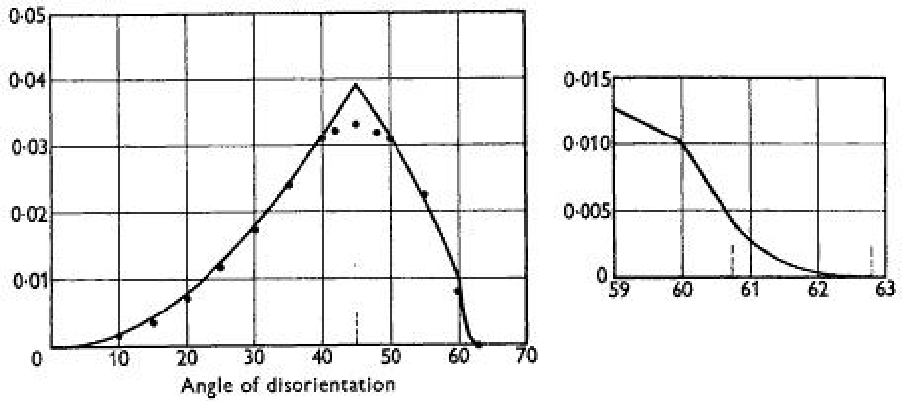

Fig. 2. The density function for the angle of disorientation. The ordinate is probability density when the angle is measured in degrees and the dots are estimates derived from random sampling.

6. Min ⟨100⟩

If α is the value of Min ⟨100⟩, then, using (3·1) and the result of § 4, it follows that

$$\sin \tfrac{1}{2}\alpha = \sin\theta \sin \tfrac{1}{2}\psi, \qquad (6\cdot 1)$$

and the probability element (5·1) becomes

$$dV(\mathbf{R}^*) = (288/\pi^2) \sin\alpha \, d\alpha \, d\beta \, d\phi, \qquad (6\cdot 2)$$

where

$$\beta = \operatorname{arsin}(t \cot\theta), \qquad (6\cdot 3)$$

$$t = \tan \tfrac{1}{2}\alpha. \qquad (6\cdot 4)$$

The density function for α is found by integrating (6·2) with respect to β and ϕ over the region determined by (4·2) and (6·1). The main difficulties are the determination of the appropriate limits of integration and the reduction of the double integrals to single integrals.

The limits of integration are determined in two steps. First, a diagram is constructed which shows the limits of the variables θ and ψ for the case where the ϕ integration is carried out first. Most of the results required to do this are available as a result of the calculations in the preceding section, the only extension necessary arising from the fact that no use can now be made of the simplifications which arose previously by the use of a pole at [111]. The second step is to use this diagram together with (6·1) to obtain the limits for θ, and hence β, when α is fixed.

The diagram is shown in Fig. 3 and the limits for ϕ in the three regions are

$$\left.\begin{aligned}
&\text{I:} && 0 \leqslant \phi \leqslant \tfrac{1}{4}\pi,\\
&\text{II:} && \arccos(\cot\theta) \leqslant \phi \leqslant \tfrac{1}{4}\pi,\\
&\text{III:} && \arccos(\cot\theta) \leqslant \phi \leqslant \tfrac{1}{4}\pi - \arccos\left[(\cot\tfrac{1}{2}\psi - \cos\theta)/\sqrt{2}\sin\theta\right],\\
& && \text{or } \arccos\left[t^{-1}\sin\beta\right] \leqslant \phi \leqslant \tfrac{1}{4}\pi - \arccos\left[t^{-1}\sin(\tfrac{1}{4}\pi - \beta)\right].
\end{aligned}\right\} \tag{6·5}$$

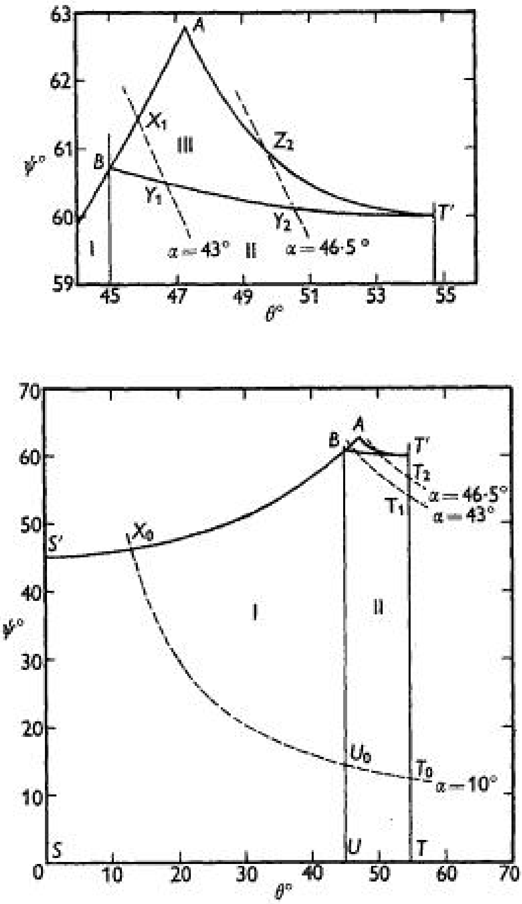

Fig. 3. Diagrams showing the limits of the variables θ and ψ when the ϕ integration is carried out first. Some typical curves with α a constant are shown dotted.

For a fixed ψ, the boundaries SS', BU and TT' are determined by the values of θ at the corresponding points in Fig. 1; the values of $\cos\theta$ are 1, $1/\sqrt{2}$ and $1/\sqrt{3}$, respectively. The boundary $S'BA$ is determined by the value of θ on the arcs P_rQ_r on Fig. 1, BT' by the value of θ at P_1' and AT' by the value of θ at Q_r'. Thus, on

$$\left.\begin{aligned}
&S'BA: & \cos\theta &= (\sqrt{2}-1)\cot\tfrac{1}{2}\psi,\\
&BT': & \cos\theta + \sqrt{2}\sin\theta &= \cot\tfrac{1}{2}\psi,\\
&AT': & \cos\theta + \sin\theta(\cos\phi + \sin\phi) &= \cot\tfrac{1}{2}\psi,\\
& & \cos\phi &= \cot\theta.
\end{aligned}\right\} \tag{6·6}$$

The dotted curves like hyperbolae drawn on Fig. 3 are curves of constant α determined by (6·1), and the change of variables implied by (6·2) means that the integration with respect to β is along these curves on the diagram. The limiting values of β are determined by the intersections of the dotted curves with the solid boundaries drawn on Fig. 3. After some calculation it is found that at

$$\left.\begin{aligned} X_r \text{ on } S'BA: &\quad \beta = \tfrac{1}{8}\pi, \\ Y_r \text{ on } BT': &\quad \beta = \tfrac{1}{4}\pi - \operatorname{arsin} t, \\ Z_r \text{ on } AT': &\quad \beta = \operatorname{arsin}\,[t\cos(\tfrac{1}{8}\pi+\gamma)], \\ T_r \text{ on } TT': &\quad \beta = \operatorname{arsin}\,(t/\sqrt{2}), \\ U_r \text{ on } UB: &\quad \beta = \operatorname{arsin} t, \end{aligned}\right\} \tag{6·7}$$

where
$$\sin^2\gamma = [(\sqrt{2}+1)^2 t^2 - 1]/4\sqrt{2}\,t^2. \tag{6·8}$$

Clearly there are three ranges of α to be considered according as the curve α = constant intersects $S'B$, BA or AT' when the subscript r in (6·7) takes the values 0, 1 or 2, respectively.

The required integrals are all reduced in much the same way and only the case where the curve α = constant intersects $S'B$ will be treated; in this case

$$0 \leqslant \tan\tfrac{1}{2}\alpha \leqslant [(\sqrt{2}-1)/2\sqrt{2}]^{\frac{1}{2}}, \quad \text{or} \quad 0 \leqslant \alpha \leqslant 41{\cdot}88^\circ.$$

Using Fig. 3, (6·5), and (6·7), the required double integral is written down and the integration over ϕ carried out first. Then the term $\operatorname{arcos}(t^{-1}\sin\beta)$ arising from this integration is immediately replaced by an integral again. Omitting the factor $(288/\pi^2)\sin\alpha$, the result at this stage is

$$\tfrac{1}{4}\pi\int_{\operatorname{arsin}(t/\sqrt{2})}^{\frac{1}{8}\pi} d\beta - \int_{\operatorname{arsin}(t/\sqrt{2})}^{\operatorname{arsin} t} d\beta \int_0^{\operatorname{arcos}(t^{-1}\sin\beta)} d\phi. \tag{6·9}$$

Finally, inverting the order of integration in the second integral and evaluating gives the result

$$\tfrac{1}{32}\pi^2 - \int_0^{\frac{1}{4}\pi} \operatorname{arsin}\,(t\cos\phi)\,d\phi. \tag{6·10}$$

The same result (6·10) is obtained for the next range of α, but a different result is obtained in the third range of α. When α is measured in degrees, the required density function is

$$p(\alpha) = (8/5\pi)\sin\alpha\left[\tfrac{1}{32}\pi^2 - \int_0^{\frac{1}{4}\pi} \operatorname{arsin}\,(t\cos\phi)\,d\phi\right], \tag{6·11}$$

when $0 \leqslant \alpha \leqslant 45^\circ$ and

$$p(\alpha) = (8/5\pi)\sin\alpha\left[\tfrac{1}{32}\pi^2 - \int_0^{\frac{1}{4}\pi} \operatorname{arsin}\,(t\cos\phi)\,d\phi - \tfrac{1}{4}\pi\gamma + \int_{\frac{1}{8}\pi-\gamma}^{\frac{1}{8}\pi+\gamma} \operatorname{arsin}\,(t\cos\phi)\,d\phi\right], \tag{6·11'}$$

when $45^\circ \leqslant \alpha \leqslant \operatorname{arcos}\frac{2}{3} = 48{\cdot}19^\circ$ and where

$$\left.\begin{aligned} t &= \tan\tfrac{1}{2}\alpha, \\ \sin^2\gamma &= [(\sqrt{2}+1)^2 t^2 - 1]/4\sqrt{2}\,t^2. \end{aligned}\right\} \tag{6·12}$$

For small α, equation (6·11) gives $p(\alpha) = (\frac{1}{180}\pi)\, 9 \sin\alpha$, in agreement with the estimate made by Mackenzie & Thomson (1957).

Both the density function and its cumulative distribution function have been computed and the results are given in Table 2 and Fig. 4. The density function and its first derivative are continuous at $\alpha = 45°$, but the second derivative is discontinuous there. The dots on

Table 2. *Distribution of angle* Min ⟨100⟩

$\alpha°$	$p(\alpha)$	C.D.F.†	$\alpha°$	$p(\alpha)$	C.D.F.†
0	0·00000	0·00000	45	0·00290	0·99723
5	·01232	·03196	46	·00119	·99917
10	·02180	·11846	47	·00033	·99987
15	·02835	·24508	48	·00001	1·00000
20	·03191	·39701	48·18...	·00000	1·00000
25	0·03241	0·55910			
30	·02980	·71591			
35	·02403	·85181			
40	·01508	·95093			
45	·00290	·99723			

† C.D.F. = cumulative distribution function.

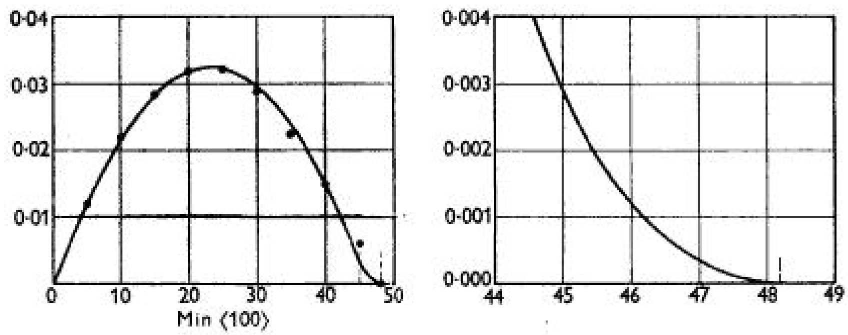

Fig. 4. The density function for the angle Min ⟨100⟩. The ordinate is probability density when the angle is measured in degrees and the dots are estimates derived from random sampling.

Fig. 4 give a graphically smoothed estimate of the density function obtained from the random sampling calculations and again the agreement with the true density function is better than would have been expected. The mean, standard deviation, median and the mode were calculated to be

$$\left.\begin{aligned} \bar{\alpha} &= 23{\cdot}164°, \\ \sigma &= 10{\cdot}312°, \\ \alpha_{\mathrm{med.}} &= 23{\cdot}183°, \\ \alpha_{\mathrm{mode}} &= 23{\cdot}308°. \end{aligned}\right\} \quad (6{\cdot}13)$$

The integrals in (6·11) were evaluated by direct numerical integration while the integral in (6·10) was calculated from the power series

$$\sqrt{2}\int_0^{\frac{1}{4}\pi} \operatorname{arsin}(t\cos\phi)\,d\phi = \sum_{r=0}^{\infty} a_{2r+1}t^{2r+1}, \tag{6·14}$$

where

$$\left.\begin{aligned} a_1 = 1, \quad a_3 = 5/36, \quad a_5 = 43/800, \quad a_7 = 177/6272,\\ a_9 = 2867/165{,}888, \quad a_{11} = 11{,}531/991{,}232,\\ a_{13} = 92{,}479/11{,}075{,}584, \quad a_{15} = 74{,}069/11{,}796{,}480. \end{aligned}\right\} \tag{6·15}$$

In the neighbourhood of $\alpha = 45°$ the behaviour of the density function is given by

$$p(\alpha) = p_-(\alpha) = 0{\cdot}002896 - 0{\cdot}002763x - 0{\cdot}000070x^2, \tag{6·16}$$

for $x = 45 - \alpha$ negative and

$$p(\alpha) = p_+(\alpha) = p_-(\alpha) + 0{\cdot}001107x^{\frac{3}{2}} + 0{\cdot}000018x^{\frac{5}{2}}, \tag{6·17}$$

for x positive. Near the limit of the distribution at $\alpha = 48{\cdot}19°$

$$p(\alpha) = 0{\cdot}000217(\alpha - 48{\cdot}19)^2, \tag{6·18}$$

in agreement with the behaviour predicted by Mackenzie & Thomson (1957).

I wish to thank Mr D. C. Handscomb for communicating to me the final result for the density function for the angle of disorientation.

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