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STEREOLOGY OF DIHEDRAL ANGLES

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Abstract. The paper presents a short survey of stereological problems concerning dihedral angles, their solutions and applications, and introduces a graph for determining the distribution functions of planar angles under the hypothesis that dihedral angles in $\mathbb{R}^3$ are of the same size and create a random field.

Keywords: dihedral angles, distribution function, graph theory, stereology

MSC 2000: 60D05, 52A22

1. Introduction

The first paper showing the importance of dihedral angles from the point of view of the characterization and behaviour of metallic materials was published by Harker and Parker [8]. They calculated the distribution function $H_{\chi^\circ}(x^\circ)$ of a random variable ψ°, taking the values x° of planar angles (in degrees) observable in a random planar section, under the hypothesis of an ideal stable spatial structure characterized by dihedral angles of the same size $\chi^\circ = 120^\circ$ only. Riegger and van Vlack [12] plotted the graphs of $H_{\chi^\circ}(x^\circ)$ for further predetermined values of χ° angles (from $\chi^\circ = 15^\circ$ to 165° [15°]). All these curves were obtained by numerical integration of areas on a map of ψ° angles constructed by Harker and Parker [8]. Duvaljan [7] was the first to consider χ° as a random variable and suggested an approximate formula for the conditional variance $\mathrm{var}(\psi^\circ|\chi^\circ)$. Duvaljan's results were applied by Rys and Kasperczyk [13] to the investigation of metal and alloy microstructure heterogeneity and were widely discussed by Schwandtke [14]. DeHoff [6] estimated the expected value $E(\chi^\circ)$ in terms of the area point count and of the tangent count, but Brakke [1] showed that this estimator is of low precision, especially for small angles. Miles

[10] presented the probability density function $g_o(u)$ of $u = \cot\chi$ as a solution of a Fredholm integral equation of the first kind with a symmetric kernel. The analytical forms of the distribution function $H_{\chi^\circ}(x^\circ)$ and the probability density $h_{\chi^\circ}(x^\circ)$ of planar angles ψ° under the hypothesis of a random field of constant dihedral angle χ° in $\mathbb{R}^3$ were derived by Reeds and Butler [11] in connection with solving physiological problems concerning the investigation of optical properties of lungs (Butler et al. [3], Suzuki et al. [15]). The mathematical formulation of the dihedral angle problems together with the above mentioned formula for $H_{\chi^\circ}(x^\circ)$ found by Reeds and Butler [11] are recalled in Section 2 of this paper. To facilitate the use of this formula in practice we decided to apply the graphical method. It enables us to determine the distribution function $H_{\chi^\circ}(x^\circ)$ for a fixed but arbitrary value of the dihedral angle χ° and is introduced in Section 3 of this paper. Analogous graphs for determining the probability density function $h_{\chi^\circ}(x^\circ)$ have been already constructed and published by Horálek [9].

2. Dihedral angle and the distribution function of its random planar sections

An edge C_i is defined as an intersection of two surfaces $Y_{2(1)}$ and $Y_{2(2)}$. Such a situation can arise in space as well as in situations where more than two surfaces are meeting as e.g. in a cell structure with space-filling grains (polyhedrons); here a grain edge is created by the intersection of boundaries of adjoining grains.

Let us suppose that at each point $c \in C_i$ two planes tangential to C_i exist and these planes are tangential also to the smoothly varying surfaces at the point c. Each pair of adjoining tangential half-planes creates a wedge W smoothly varying as the point c continuously traverses C_i. The angle of the wedge W at the point c is the dihedral angle $\chi(c)$ or briefly χ, $0 < \chi < \pi$.

For simplicity, let us consider only two surfaces $Y_{2(1)}$ and $Y_{2(2)}$. The intersection of the corresponding two tangential half-planes T_{W1} and T_{W2} creates a tangent to the edge C_i at the point c. The true size of the dihedral angle at $c \in C_i$ is observable only in a plane normal to this tangent and such a plane creates an orthogonal section of the dihedral angle. This situation is illustrated in Fig. 1.

Let the wedge W bounded by the half-planes T_{W1} and T_{W2} have a fixed angle χ. Intercepting this wedge by a random plane T_2, the half-lines $T_2 \cap T_{W1}$ and $T_2 \cap T_{W2}$ form in T_2 an angle ψ $(0 < \psi < \pi)$ the size of which depends on the orientation of T_2. In general, the equality $\psi = \chi$ is fulfilled only when T_2 is an orthogonal section plane ($\chi = \pi/2$ is an exceptional case). In all other cases, ψ is a random variable.

Now consider a random field of dihedral angles in the $\mathbb{R}^3$ space, these angles of the same size having random positions and orientations, i.e. at least one of the

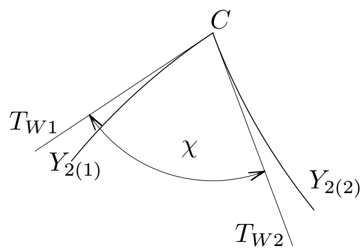

Figure 1. Orthogonal section of the dihedral angle χ.

probability distributions of the dihedral angle or of the section plane T_2 should be isotropic. In the section plane T_2 we observe only induced images of χ and therefore the corresponding moments of the random variable ψ are only conditional mean values and the distribution function of ψ is only a conditional distribution function.

Let (x, y, z) be the cartesian coordinates in $\mathbb{R}^3$, let the plane T_2 intersect the z-axis at the point $(0, 0, z)$ and let the direction vector of T_2 be a point r in the upper unit hemisphere

$$r = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$$

for $0 < \theta < \pi/2$, $0 < \varphi < 2\pi$, $-\infty < z < \infty$—see Fig. 2.

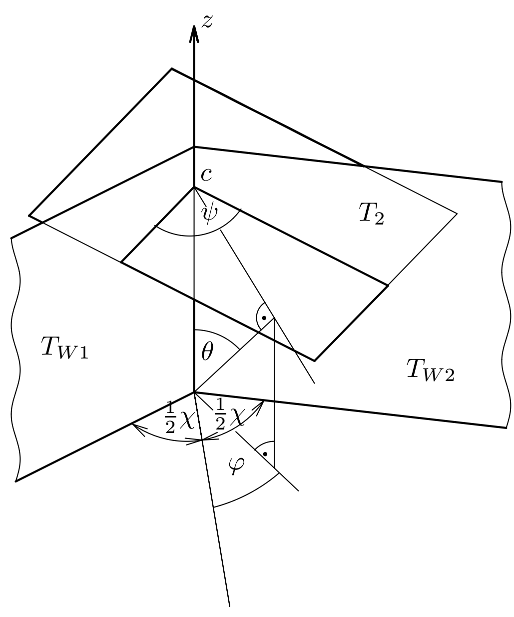

Figure 2. Section of the wedge W bounded by the half-planes T_{W1}, T_{W2}, by the plane T_2.

Then provided T_2 intersects the edge $C_i \subset z$ at c, or more precisely expressed, that T_2 intersects a linear element ΔC_i of the edge C_i, the marginal orientation density is given by

$$f(\theta, \varphi \mid T_2 \uparrow \Delta C_i) = \frac{1}{\pi} \sin\theta \cos\theta = \frac{1}{2\pi} \sin 2\theta.$$

When rotating T_2 in such a way that $c \in C_i$ remains fixed and the angle θ is constant, only φ varies. Since φ is uniformly distributed on $(0, 2\pi)$, the probability that a half-line starting from c in T_2 lies in the dihedral angle χ is equal to $\chi/(2\pi)$.

Reeds and Butler [11] have derived the conditional distribution function

$$H_a(b) = \Pr(\cos\psi < b \mid \chi), \tag{1}$$

where

$$a = \cos\chi. \tag{2}$$

We have

$$H_a(b) = \begin{cases} \dfrac{\chi}{\pi} - 8L(b, a)\dfrac{1}{\pi \sin\chi} & \text{for } a \leqslant b \\ \dfrac{\chi}{\pi} + 8L(-b, -a)\dfrac{1}{\pi \sin\chi} & \text{for } b \leqslant a, \end{cases} \tag{3}$$

where

$$\begin{aligned} L(b, a) = C(b, a)[&3(1 + b)(1 - a)R_F(x, y, 1) - b(1 + a)R_D(y, 1, x) \\ &- b(1 - b)R_D(1, x, y) + b(b - a)R_D(x, y, 1) \\ &+ 2aR_J(x, y, 1, w)] + \frac{b(1 - b)(1 + a)^2}{4(1 - a)(1 + b)^2} \end{aligned}$$

and

$$C(b, a) = -\frac{(b - a)(1 + a)}{6(1 - a)^{3/2}(1 + b)^{5/2}}.$$

The Carlson elliptic integrals $R_F(x, y, z)$, $R_D(x, y, z)$ and $R_J(x, y, z, w)$ are defined for positive distinct x, y, z and w as follows (Carlson [4]):

$$R_F(x, y, z) = 0.5 \int_0^\infty \frac{1}{Q^{1/2}}\, \mathrm{d}v, \qquad R_D(x, y, z) = 1.5 \int_0^\infty \frac{1}{(v + z)Q^{1/2}}\, \mathrm{d}v,$$

$$R_J(x, y, z, w) = 1.5 \int_0^\infty \frac{1}{(v + w)Q^{1/2}}\, \mathrm{d}v,$$

where

$$Q = (v + x)(v + y)(v + z)$$

and the arguments x, y and w are functions of a and b introduced in (2) and (3), respectively,

$$x = \frac{b-a}{1-a}, \quad y = \frac{b-a}{1+b} \qquad \text{and} \qquad w = \frac{2(b-a)}{(1-a)(1+b)}.$$

3. Graph for determining the conditional distribution function $H_{\chi^\circ}(x^\circ)$

In contrast to (1), in order to simplify the use of the graph in practice, we consider here the conditional distribution function

$$H_{\chi^\circ}(x^\circ) = \Pr(\psi^\circ \leqslant x^\circ \mid \chi^\circ = \text{const}),$$

where the angles χ°, ψ° are given in degrees. The construction of the graph in Fig. 3 is based on quantiles $x^\circ{}_P$ fulfilling the equation

$$H_{\chi^\circ}(x^\circ_P) = P(\chi^\circ).$$

The values $x^\circ{}_P$ were calculated for $P(\chi^\circ) = 0.005; 0.01; 0.03; 0.05; 0.1; 0.2, \ldots, 0.9; 0.95; 0.97; 0.99$ and 0.995 and for $\chi^\circ = 2.5^\circ$ to 90° $[2.5^\circ]$; the tables of this quantiles will be published separately. For preparing the computer program the computer routines for Carlson elliptic integrals elaborated by Carlson and Notis [5] were employed.

The shapes of isocurves $P(\chi^\circ)$ are plotted in Part A of Fig. 3 separately for $0 < \chi^\circ \leqslant 90^\circ$ and for $90^\circ < \chi^\circ \leqslant 180^\circ$, respectively; it should be noted that only the values of χ° and of P, that have the same orientation of the legend are related mutually. The property of the distribution function $H_a(b)$, defined in (1), namely

$$H_{-a}(-b) = 1 - H_a(b), \tag{4}$$

was taken into account.

For a fixed but arbitrary angle χ° $(0 < \chi^\circ < 180^\circ)$, the corresponding $H_{\chi^\circ}(x^\circ)$ can be constructed in agreement with the key drawn in the graph. The point of intersection of a horizontal straight line at an arbitrary angle value χ° with the chosen quantile isocurve $P(\chi^\circ)$—see Fig. 3, Part A—determines uniquely the quantile $x^\circ{}_P$ for which the distribution function $H_{\chi^\circ}(x^\circ{}_P)$ takes the value $P(\chi^\circ)$—see Fig. 3, Part B. In this way, we are able to determine 17 points of the distribution function $H_{\chi^\circ}(x^\circ)$.

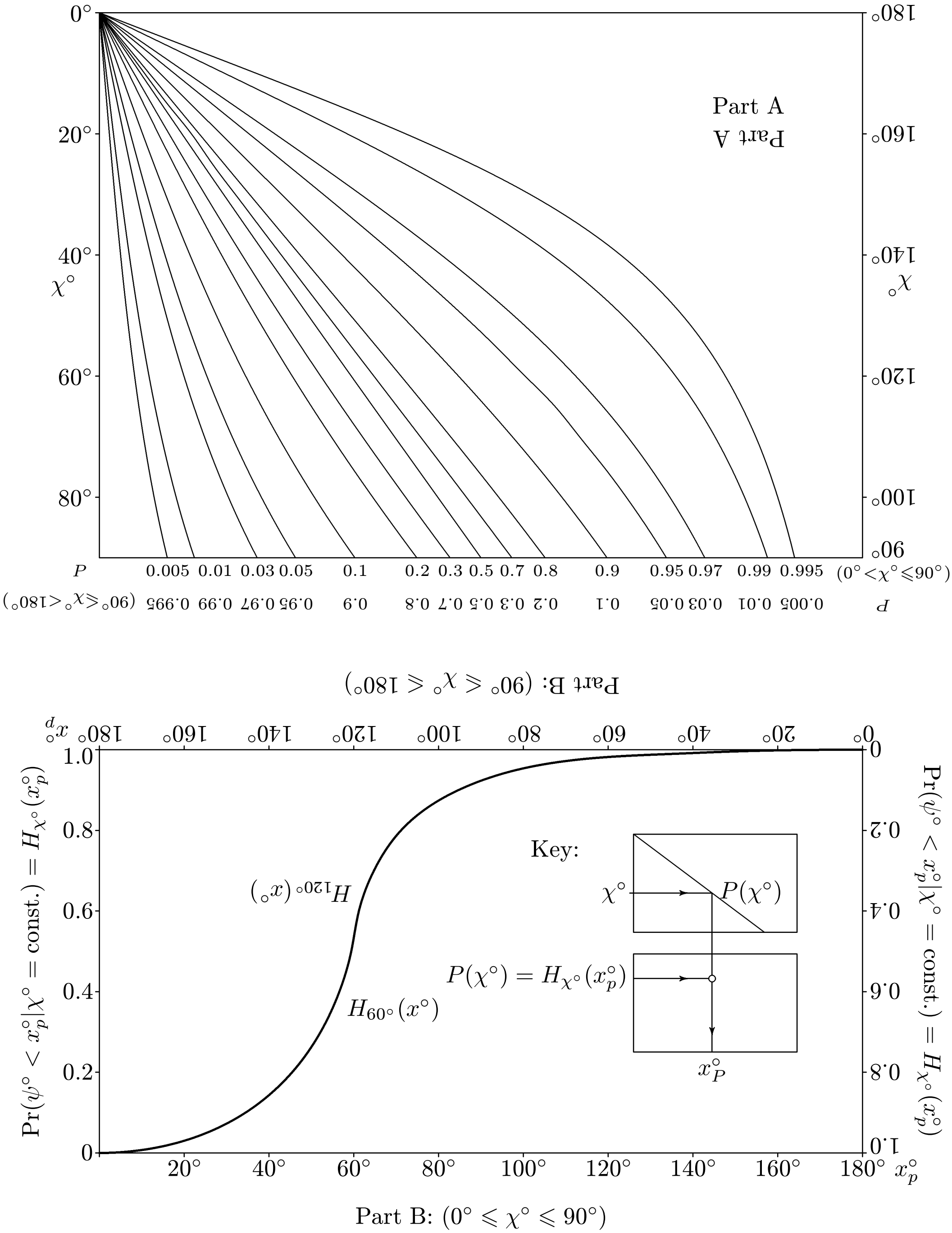

Figure 3. Graph for determining the conditional distribution function $H_{\chi°}(x°)$.

To illustrate the above outlined procedure, let us assume the dihedral angle $\chi^\circ = 60^\circ$ forming a random field in $\mathbb{R}^3$. The relevant $H_{60^\circ}(x^\circ)$ of the random variable ψ°, $0^\circ < \psi^\circ < 180^\circ$, taking the values of induced images of the dihedral angle χ° observable in the section plane T_2, is presented in Part B of Fig. 3. For determining $H_{120^\circ}(x^\circ)$, we have used the relationship following from (4). Of course, $H_{0^\circ}(0^\circ) = 0$ and $H_{180^\circ}(180^\circ) = 1$.

The knowledge of the graphical course of $H_{\chi^\circ}(x^\circ)$ permits to test the hypothesis on χ° by using the empirical distribution function of planar angles measured in the section plane T_2, i.e. to apply a graphical form of a test of goodness of fit, e.g. the Kolmogorov-Smirnov test, to the measurement results plotted in the graph, and to verify the hypothesis that all dihedral angles are of the same size the value of which can be estimated by the average of planar angles observed in the plane section.

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