Textures and Microstructures, Vol. 33, pp. 365–373
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Printed in Malaysia.

THE DE LA VALLÉE POUSSIN STANDARD ORIENTATION DENSITY FUNCTION

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The de la Vallée Poussin standard orientation density function $\mathcal{V}_\kappa(\omega) = C(\kappa)\cos^{2\kappa}(\omega/2)$ is discussed with emphasis on the finiteness of its harmonic series expansion which advantageously distinguishes it from other known standard functions. Given its halfwidth, the de la Vallée Poussin standard orientation density function allows, for example, to tabulate the degree of series expansion into harmonics required for its exact representation.

Keywords: Integral equation of texture goniometry; Spherical X-ray transform; Invariance of distribution type; de la Vallée Poussin type of distribution; von Mises–Fisher distribution

1 INTRODUCTION: ODFs AND DIFFRACTION PDFs

1.1 Standard Functions

A standard orientation density function should satisfy the requirements (i) to be specified by a small number of parameters, (ii) mathematically and numerically tractable, (iii) generally appealing from the point of physical interpretation, and (iv) possess analytical expressions for corresponding pole density functions and all normalization constants thus avoiding truncation errors (Matthies *et al.*, 1987). All these requirements are satisfied by the hyperspherical de la Vallée Poussin type density function

$$\mathcal{V}_\kappa(\omega) = \frac{B(\frac{3}{2},\frac{1}{2})}{B(\frac{3}{2},\kappa+\frac{1}{2})}\cos^{2\kappa}(\omega/2),\ \omega\in[0,\pi],\ \kappa\in\mathbb{N}\cup\{0\},\ \kappa_0=\infty \quad (1)$$

which includes for $\kappa = 0$ the uniform distribution and converges for $\kappa \to \kappa_0$ to the δ-distribution; $B(\alpha, \beta)$ denotes the Beta-function. The de la Vallée Poussin type orientation density function has first been discussed in (Schaeben, 1996; 1997). Standard functions are used to study "ghost effects" caused by the ambiguity of the inverse problem of texture goniometry, and are applied in texture component fit methods where they represent components of preferred crystallographic orientation to be fitted to experimental pole intensities.

1.2 Projection Equation of Texture Goniometry

Mathematical texture analysis used to be primarily concerned with the resolution of the tomographic inverse problem corresponding to the fundamental projection equation of diffraction texture goniometry as follows.

Let $f \in \mathcal{L}^2(G)$, $G \subset \mathrm{SO}(3)$, be a square integrable function defined on an appropriate subgroup G of the group SO(3) of orientations, i.e. proper rotations for the three-dimensional space $\mathbb{R}^3$. Let $S^3 \subset \mathbb{R}^3$ denote the unit sphere in the three-dimensional space, and let $\mathbf{v}, \mathbf{u} \in S^3$, then the integral operator $\mathcal{P}_\mathbf{v}$: $\mathcal{L}^2(G) \to \mathcal{L}^2(S^3)$ is defined as

$$\mathcal{P}_\mathbf{v}[f(g)](\mathbf{u}) = (\mathcal{P}_\mathbf{v} f)(\mathbf{u}) = \frac{1}{2\pi} \int_{\{g \in G \mid \mathbf{v} = g\mathbf{u}\}} f(g) \mathrm{d}g = P_\mathbf{v}(\mathbf{u}). \tag{2}$$

The function $P_\mathbf{v}$ may be referred to as (hyper)spherical X-ray transform of f as it represents the one-dimensional line integrals of f, (Louis and Natterer, 1983). Obviously, $P_{-\mathbf{v}}(\mathbf{u}) = P_\mathbf{v}(-\mathbf{u})$; however generally $P_\mathbf{v}(\mathbf{u}) \neq P_\mathbf{v}(-\mathbf{u})$.

A crystallographic pole density function $\tilde{P}_h$ of the crystal form $h = \{\mathbf{h}_m \mid m = 1, \ldots, M_h\} \subset S^3$ with multiplicity M_h corresponding to symmetrically equivalent lattice planes $\{(hkl)_m \mid m = 1, \ldots, M_h\} \subset \mathbb{Z}^3$ is defined as superposition of the X-ray transforms of a crystallographic orientation density function $f \in \mathcal{L}^2(G)$ for the directions $h = \{\mathbf{h}_m \mid m = 1, \ldots, M_h\}$. Since $\mathbf{h}_m \in h$ always induces $-\mathbf{h}_m \in h$, a crystallographic pole density function is an even function, i.e.

$$\tilde{P}_h(\mathbf{r}) = \tilde{P}_h(-\mathbf{r}). \tag{3}$$

1.3 Path of Integration

Applying the Rodrigues parametrization of rotations, i.e. representation by quaternions, the set $\{g \in SO(3) \mid g\mathbf{u} = \mathbf{v}\}$ may be represented as the circle on the unit sphere $S_+^4 \subset \mathbb{R}^4$ given by

$$\mathbf{q}(t) = \mathbf{q}_1 \cos(t/2) + \mathbf{q}_2 \sin(t/2), \quad t \in [-\pi, \pi] \tag{4}$$

where for (i) $\mathbf{u} \neq -\mathbf{v}$

$$\mathbf{q}_1 = \begin{pmatrix} n_{11}\sin(\zeta/2) \\ n_{12}\sin(\zeta/2) \\ n_{13}\sin(\zeta/2) \\ \cos(\zeta/2) \end{pmatrix}, \qquad \mathbf{q}_2 = \begin{pmatrix} n_{21} \\ n_{22} \\ n_{23} \\ 0 \end{pmatrix} \tag{5}$$

with either

$$\cos\zeta = \mathbf{uv}, \qquad \mathbf{n}_1 = \frac{1}{\sin\zeta}(\mathbf{v} \times \mathbf{u}) \in S^3 \tag{6}$$

if $\mathbf{u} \neq \mathbf{v}$, or

$$\zeta = 0, \qquad \mathbf{n}_1 = \mathbf{u} \tag{7}$$

if $\mathbf{u} = \mathbf{v}$, and

$$\mathbf{n}_2 = \frac{1}{2\cos(\zeta/2)}(\mathbf{v} + \mathbf{u}) \in S^3 \tag{8}$$

or for (ii) $\mathbf{u} = -\mathbf{v}$

$$\mathbf{q}_1 = \begin{pmatrix} q_{11} \\ q_{12} \\ q_{13} \\ 0 \end{pmatrix}, \qquad \mathbf{q}_2 = \begin{pmatrix} q_{21} \\ q_{22} \\ q_{23} \\ 0 \end{pmatrix} \tag{9}$$

with two linearly independent $(q_{11}, q_{12}, q_{13})^t, (q_{21}, q_{22}, q_{23})^t \in S^3$ orthogonal to $\mathbf{u}$.

Equation (2) may then be rewritten as

$$P_{\mathbf{v}}(\mathbf{u}) = \frac{1}{2\pi}\int_{(-\pi,\pi)} f(\mathbf{q}(t))\,\mathrm{d}t, \tag{10}$$

where $\mathrm{d}t$ denotes the measure of the one-dimensional circle restricted to S_+^4.

As $\mathbf{q}(t)$ varies according to Eq. (4), the corresponding angle of rotation $\omega(t)$ varies for $\mathbf{u} \neq \pm\mathbf{v}$ according to

$$q_4(t) = \cos\frac{\zeta}{2}\cos\frac{t}{2} = \cos\frac{\omega(t)}{2}, \quad t \in [-\pi, \pi]. \tag{11}$$

Equation (10) proves useful for analytical integration of (2).

2 DE LA VALLÉE POUSSIN STANDARD ORIENTATION DENSITY FUNCTION

Let an orientation density function f rotationally invariant with respect to g_0 be given by the hyperspherical de la Vallée Poussin type density function

$$f(g; g_0, \kappa) = \mathcal{V}_\kappa(\omega) = \frac{B(\frac{3}{2},\frac{1}{2})}{B(\frac{3}{2},\kappa+\frac{1}{2})}\cos^{2\kappa}(\omega/2),$$
$$\omega = \omega(g_0^{-1}g) \in [0,\pi], \quad \kappa \in \mathbb{N} \cup \{0\}. \tag{12}$$

Its coefficients C_l according to the expansion

$$\mathcal{V}_\kappa(\omega) \doteq \sum_{l=0}^{\infty} C_l(\kappa)\frac{\sin((2l+1)\omega/2)}{\sin(\omega/2)} \tag{13}$$

into even-order Chebychev polynomials of second kind are given by

$$C_l(\kappa) = \frac{2}{\pi}\int_{[0,\pi]} \mathcal{V}_\kappa \frac{\sin((2l+1)\omega/2)}{\sin(\omega/2)}\sin^2\frac{\omega}{2}\,\mathrm{d}\omega$$
$$= \frac{1}{2B(\frac{3}{2},\kappa+\frac{1}{2})}[\mathcal{I}_l(\kappa) - \mathcal{I}_{l+1}(\kappa)], \quad l = 0, 1, \ldots \tag{14}$$

with

$$\mathcal{I}_l(\kappa) = \sum_{k=0}^{l} (-1)^k \binom{2l}{2k} B(k+\frac{1}{2}, \kappa + l - k + \frac{1}{2}), \quad l = 0, 1, \ldots . \tag{15}$$

Obviously, the coefficients C_l eventually vanish, that is $C_l(\kappa) = 0$ for $l > \kappa$. Thus, the infinite series (13) reduces to a finite series, such that truncation is not required in practical numerical applications involving C_l coefficients and errors due to truncation are avoided. This property essentially distinguishes the de la Vallée Poussin standard orientation density function from the other known standard functions of von Mises-Fisher-, Cauchy-, or Brownian-type in an advantageous way.

For the de la Vallée Poussin standard orientation density function its parameter κ and its halfwidth b, with $b = 2\omega_b$, are related through

$$\cos^{2\kappa}\left(\frac{\omega_b}{2}\right) = \frac{1}{2} \tag{16}$$

which implies

$$\omega_b = 2 \arccos\left(\left(\frac{1}{2}\right)^{1/2\kappa}\right) \tag{17}$$

or

$$\kappa = \frac{1}{2} \frac{\ln(1/2)}{\ln(\cos(\omega_b/2))}. \tag{18}$$

Table I compiles corresponding values of the halfwidth b and the concentration parameter κ, visualized in Fig. 1. Since κ may also be read as the degree of the harmonic series expansion required to exactly represent the de la Vallée Poussin standard orientation density function by hyperspherical harmonics, Table I indicates that it takes, e.g. a total of 40(80) C coefficients to do so for a moderate degrees of preferred crystallographic orientation given by a halfwidth b roughly equal to 30(20); for b roughly equal to 10, a total of 364 terms of the harmonic series expansion are required for an exact representation.

TABLE I Corresponding values of halfwidth b and harmonic series expansion degree κ required for exact representation

b	κ	b	κ
84.35	5	20.10	90
59.99	10	19.07	100
49.08	15	17.06	125
42.54	20	15.57	150
38.07	25	14.42	175
34.77	30	13.49	200
32.20	35	12.06	250
30.13	40	11.01	300
28.41	45	10.20	350
26.95	50	9.54	400
24.61	60	8.53	500
22.79	70	6.03	1000
21.32	80	4.93	1500

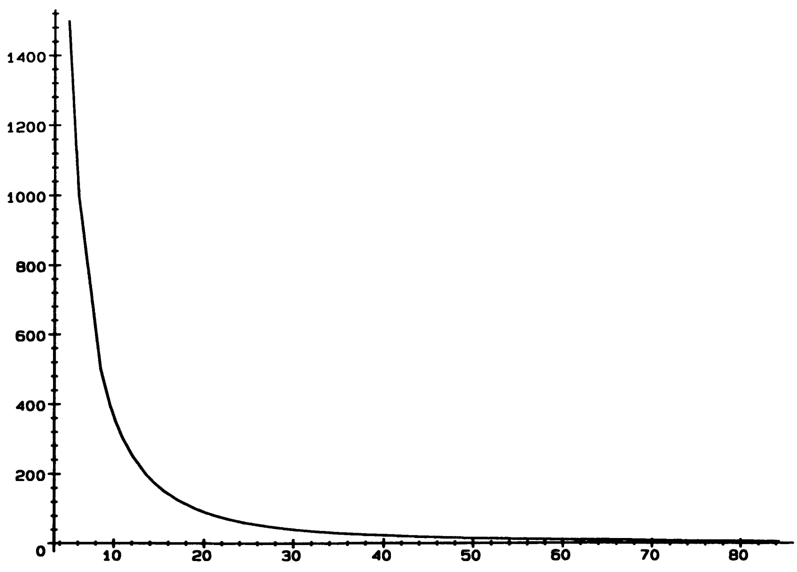

FIGURE 1 Series expansion degree κ required for exact representation vs. halfwidth b of de la Vallée Poussin standard orientation density function.

Applying the pole figure projection operator (2) and Eq. (11) yields

$$\mathcal{P}_{\mathbf{v}}[\mathcal{V}_\kappa(\omega)](\mathbf{u}) = \left\{ \frac{B(\frac{3}{2},\frac{1}{2})}{B(\frac{3}{2},\kappa+\frac{1}{2})} \frac{1}{2\pi} \int_{-\pi}^{\pi} \cos^{2\kappa}(t/2)\,\mathrm{d}t \right\} \cos^{2\kappa}(\eta/2)$$

$$= \frac{B(\frac{1}{2},\kappa+\frac{1}{2})}{2B(\frac{3}{2},\kappa+\frac{1}{2})} \cos^{2\kappa}(\eta/2)$$

$$= \frac{1}{B(1,\kappa+1)} \cos^{2\kappa}(\eta/2) = \nu_\kappa(\eta) \tag{19}$$

with $\cos\eta = \mathbf{u}g_0^{-1}\mathbf{v}$, and thus results in functions $P_{\mathbf{v}}$ which are represented by de la Vallée Poussin type density functions ν_κ on S^3. Thus, a pole density function corresponding to a given de la Vallée Poussin type orientation density function f on S_+^4 is the superposition of de la Vallée Poussin type $P_{\mathbf{h}_m}$ on S^3 centered at $\mathbf{r}_m = g_0^{-1}\mathbf{h}_m \in S^3$, $m = 1,\ldots,M_h$.

Summarily, the de la Vallée Poussin type density function provides a rotationally invariant standard orientation density function and model pole density function, respectively.

3 GRAPHICAL COMPARISON OF COMPLETE AND TRUNCATED HARMONIC SERIES EXPANSIONS OF THE DE LA VALLÉE POUSSIN STANDARD ORIENTATION DENSITY FUNCTION

It was shown in (Schaeben, 1997) that de la Vallée Poussin and von Mises–Fisher orientation density functions agree sufficiently well for pairs of parameters matched by eye. Here, an example of halfwidth-matched de la Vallée Poussin and von Mises–Fisher standard orientation density function for $b = 27.00$ with $\kappa_{\mathrm{dlVP}} = 49.825998$, and $\rho_{\mathrm{vMF}} = 25.086687$, respectively, is displayed in Fig. 2. Moreover, complete and truncated harmonic series expansions of de la Vallée Poussin standard orientation density functions with parameters $\kappa = 500, 1000$ corresponding to halfwidths $b =$ 8.53, 6.03, respectively, are rendered in Figs. 3 and 4. They reveal that for halfwidths $b \leq 10$ the loss of peak intensity is substantial for $\kappa' \leq 40, 60$, respectively.

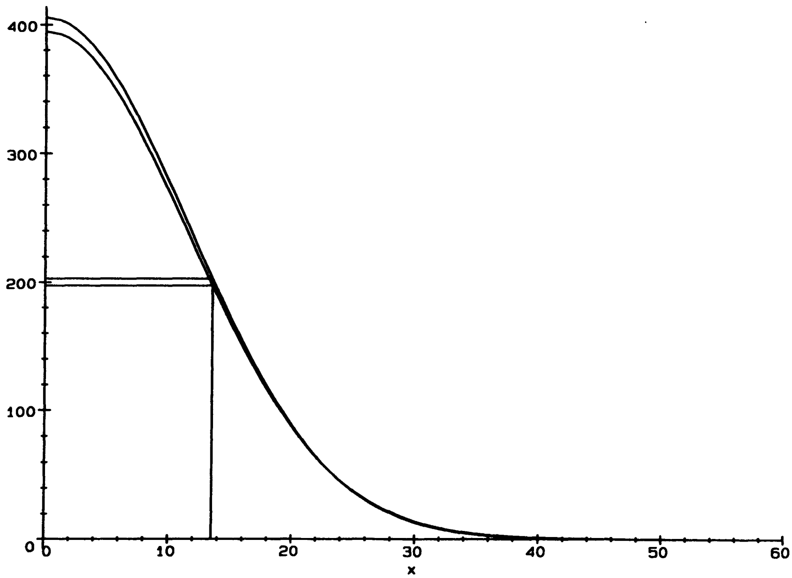

FIGURE 2 Halfwidth-matched de la Vallée Poussin (top) and von Mises–Fisher (bottom) standard orientation density function with halfwidth $b = 27$ for $\kappa_{\text{dlVP}} = 49.825998$ and $\rho_{\text{vMF}} = 25.086687$.

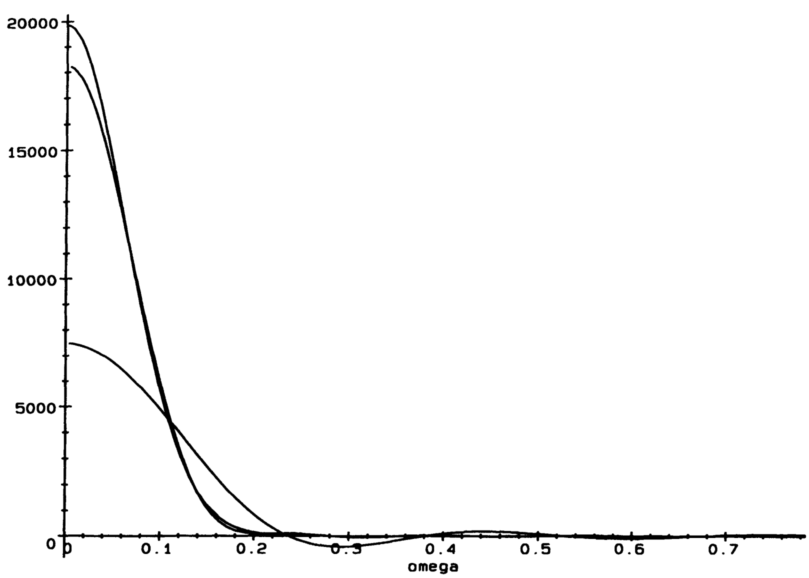

FIGURE 3 de la Vallée Poussin standard orientation density function for $\kappa = 500$ corresponding to $b = 8.53$ and its harmonic series expansion for series expansions degrees $\kappa' = 40, 20$, respectively (from top to bottom).

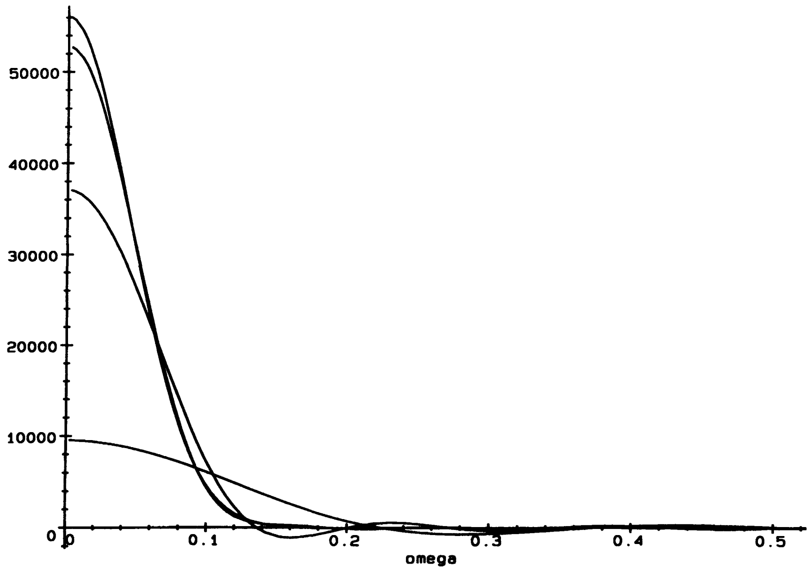

FIGURE 4 de la Vallée Poussin standard orientation density function for $\kappa = 1000$ corresponding to $b = 6.03$ and its harmonic series expansion for series expansions degrees $\kappa' = 60, 40, 20$, respectively (from top to bottom).

4 CONCLUSIONS

The de la Vallée Poussin type of distribution is preserved by the spherical X-ray transformation. For methodological fundamentals as well as for practical applications involving the harmonic C coefficients, the de la Vallée Poussin standard orientation density function is distinguished as only its first $l \leq \kappa$ coefficients C_l do not vanish.

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