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NORMAL DISTRIBUTION ON THE ROTATION GROUP SO(3)

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We study the normal distribution on the rotation group SO(3). If we take as the normal distribution on the rotation group the distribution defined by the central limit theorem in Parthasarathy (1964) rather than the distribution with density analogous to the normal distribution in Eucledian space, then its density will be different from the usual $(1/\sqrt{2\pi\sigma})$ $\exp(-(x-m)^2/2\sigma^2)$ one. Nevertheless, many properties of this distribution will be analogous to the normal distribution in the Eucledian space. It is possible to obtain explicit expressions for density of normal distribution only for special cases. One of these cases is the circular normal distribution.

The connection of the circular normal distribution SO(3) group with the fundamental solution of the corresponding diffusion equation is shown. It is proved that convolution of two circular normal distributions is again a distribution of the same type. Some projections of the normal distribution are obtained. These projections coincide with a wrapped normal distribution on the unit circle and with the Perrin distribution on the two-dimensional sphere. In the general case, the normal distribution on SO(3) can be found numerically. Some algorithms for numerical computations are given. These investigations were motivated by the orientation distribution function reproduction problem described in the Appendix.

Keywords: Normal distribution on the rotation group; Group representation; Projection; Orientation distribution function

1 INTRODUCTION

Gaussian or normally distributed random variables, Gaussian processes and systems play important roles in the theory of probability and mathematical statistics. This is due to the existence of the central limit

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theorem. This work concerns the normal distribution on the rotation group of three-dimensional space SO(3) and on the two-dimensional sphere S^2. There are many abstract works concerning probability measures (for example see Heyer (1971)), but there are few studies concerning probability distributions on specific groups, including SO(3). Mardia (1972) investigated the probability distribution on the abelian SO(2) group (unit circle) in detail and compiled some of the so-called "normal" distributions on the sphere S^2. In his book (Mardia (1972)) the normal distribution on SO(2) group is given with the probability density

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \exp\left\{ -\frac{(x+2\pi n)^2}{2\sigma^2} \right\}. \tag{1}$$

This distribution appears as a superposition of distributions on $\mathbf{R}^1$ with the equivalence relation $x_1 \equiv x_2 \,(\mathrm{mod}\, 2\pi)$. The normal distribution on SO(2) (1) satisfies the central limit theorem. Moreover the normal distribution (1) can be obtained as the solution to the diffusion equation

$$\frac{\partial f(x,t)}{\partial t} = \frac{\sigma^2}{2} \frac{\partial^2 f(x,t)}{\partial x^2} \tag{2}$$

with the initial condition in which the whole mass is concentrated at $x=0$: $f(x,0)=\delta(x)$, and the boundary condition $f(-\pi, t) = f(\pi, t)$, thus

$$f(x) = \frac{1}{\sigma\sqrt{2\pi t}} \sum_{n=-\infty}^{\infty} \exp\left\{ -\frac{(x+2\pi n)^2}{2\sigma^2 t} \right\}.$$

Another normal distribution on SO(2) was suggested by Mizes (see Mardia (1972)),

$$f(x) = \frac{1}{\sqrt{2\pi} I_0(k)} \exp\{-k\cos x\}, \quad k>0, \tag{3}$$

where $I_0(k)$ is the modified Bessel function of order 0. The normal distribution of Mizes approximates (1) and is easy to compute but does not satisfy the central limit theorem on SO(2) and is not a solution of the diffusion equation.

We will define a normal distribution on SO(3) based on Parthasarathy's work, which satisfies the central limit theorem on SO(3). Another way to define a normal distribution on SO(3) is as a solution of the corresponding diffusion equation. In this work we consider the fundamental solution of the diffusion equation on the sphere S^{n-1} in $\mathbf{R}^n$. At $n=4$ a circular normal distribution on SO(3) is obtained. At $n=3$ the normal distribution coincides with the one obtained by Perrin (1972) and Roberts and Ursell (1960) during their study of Brownian motion and random walk on S^2 in $\mathbf{R}^3$.

A normal distribution on S^2 in the present work is defined as projections corresponding to a normal distribution on SO(3). Some properties of these distributions are given. These properties of the normal distributions on SO(3) and S^2 are analogous to properties on $\mathbf{R}^n$.

Only special cases of normal distributions on SO(3) and S^2 can be calculated analytically; the rest can be found numerically. In the present work some recipes for calculating normal distributions are given. How series convergence depending on parameters of these distributions is also considered and some estimates are given.

Appendix presents an application of these normal distributions on SO(3) and S^2 to the solution of the orientation distribution function reproduction problem in the quantitative texture analysis that motivated this investigation.

2 THE NORMAL DISTRIBUTION ON SO(3) AND ITS PROPERTIES. CENTRAL LIMIT THEOREM ON SO(3)

Let us choose parametric subgroups of SO(3) $g_i(t)$, $i=1,2,3$; $0 \leq t \leq \infty$. Tangent vectors at the identity e are

$$e_i = \lim_{t \to 0} \frac{g_i(t) - e}{t}. \tag{4}$$

Let $g \to T_g^{(l)}$ denote the complete set of irreducible representations of SO(3) group (see Gelfand *et al.* (1963)). $T_g^{(l)}$ may be considered as the matrix functions on SO(3), satisfying

$$T_{g_1}^{(l)} T_{g_2}^{(l)} = T_{g_1 g_2}^{(l)},$$

where $l = 0, 1, \ldots$ are the weights of representation, and the corresponding matrix has the order $2l + 1$. Let us define an infinitesimal operator of a representation $g \longrightarrow T_g^{(l)}$, $g \in \mathrm{SO}(3)$ by

$$A_i^{(l)} = \lim_{t \to 0} \frac{T_{g_i(t)}^{(l)} - E}{t}, \tag{5}$$

where E is the identity matrix of the same order as $T_{g_i(t)}^{(l)}$.

Measure μ is said to be infinitely divisible if for every positive integer n there exist a distribution μ_n such that $\mu_n^{*n} = \mu$, where μ_n^{*n} denotes n-times convolution of the distribution μ_n. Measure μ is said to have idempotent factors if $\mu * \mu = \mu$. Define the normal distribution on the rotation group SO(3) following Parthasarathy (1967).

DEFINITION A distribution μ is said to be normal if it is infinitely divisible and without idempotent factors and for every l admits a representation

$$\int_{\mathrm{SO}(3)} T_g \, \mathrm{d}\mu(g) = \exp\left\{ \sum_{i=1}^{3} \sum_{j=1}^{3} a_{ij} A^i A^j + \sum_{i=1}^{3} a_i A^i \right\}, \tag{6}$$

where a_{ij} is a nonnegative symmetric matrix and a_i are real constants.

Consider a sequence of probability measures $\mu_n \to \delta(g)$ as $n \to \infty$, or $\lim_{n\to\infty} n\mu_n(G - U) = 0$, where U is any neighborhood of the identity, $G = \mathrm{SO}(3)$. Let us denote the "mean value" of measure μ_n as $g_n = \int_{\mathrm{SO}(3)} g \, \mathrm{d}\, \mu_n(g)$.

THEOREM 1 *If $n(1 - \det(g_n))$ is bounded as $n \to \infty$,*

$$\lim_{n\to\infty} n(e - g_n) = Q = (q_{ij}), \tag{7}$$

then any limit μ_n^{*n} is normal with parameters a_{ij}, a_i defined by the expressions

$$\begin{aligned} a_i &= 1/2(q_{jk} - q_{kj}), \quad i, j, k = 1, 2, 3, \ i \neq j \neq k, \ j > k, \\ a_{ii} &= 1/2(q_{ii} - q_{jj} - q_{kk}, \quad i \neq k, \\ a_{ij} &= -1/2(q_{ij} + q_{ji}). \end{aligned} \tag{8}$$

Proof of that theorem follows from Parthasarathy (1967) and Wehn (1962).

To find the normal distribution $d\mu(g)$ from (6) with parameters (7) and (8) we should use an inversion of the Fourier transform in the case when a probability measure is absolutely contiguous with density $f(g)$: $d\mu(g) = f(g)dg$ here dg is the invariant measure on SO(3). In that case the density allows the expansion

$$f(g) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} C_l^{mn} T_l^{mn}(g), \tag{9}$$

with the basis $\{T_l^{mn}(g)\}$ that corresponds to the unitary representation of the SO(3) group. The series (9) converges contiguously and proportionally to the nonnegative function $f(g)$ (Grenander (1963)). The matrix of the irreducible representation with weight l, in a canonical basis has the form

$$T_g^{(l)} = (T_l^{mn}(\alpha, \beta, \gamma)),$$
$$l = 0, 1, \ldots; \quad m, n = -l, -l+1, \ldots, 0, \ldots, l-1, l,$$

where $g = \{\alpha, \beta, \gamma\}$ is an arbitrary rotation with α, β, γ indicating Euler angles of rotation ($0 \le \alpha,\ \gamma < 2\pi,\ 0 \le \beta \le \pi$); and $T_l^{mn}(g)$ are generalized spherical harmonics of order l:

$$T_l^{mn}(\alpha, \beta, \gamma) = \exp\{im\alpha\} P_l^{mn}(\cos\beta) \exp\{in\gamma\},$$

$$P_l^{mn}(x) = \frac{(-1)^{l-m} i^{n-m} ((l-m)!(l+n)!)^{1/2}}{2^l (l-m)!((l+m)!(l-n)!)^{1/2}}$$
$$\times (1-x)^{-(n-m)/2} (1+x)^{-(n+m)/2}$$
$$\times \frac{d^{(l-n)}}{dx^{(l-n)}} ((1-x)^{l-m}(1+x))^{l+m},$$

where $x = \cos\beta$ and $P_l^{mn}(x)$ are the Jacobi polynomials (Vilenkin (1968)).

Let parameter subgroups of SO(3) be

$$g_1(t) = \begin{pmatrix} 1 & 0 & 0 \\ 1 & \cos t & -\sin t \\ 0 & \sin t & \cos t \end{pmatrix}, \quad g_2(t) = \begin{pmatrix} \cos t & 0 & -\sin t \\ 0 & 1 & 0 \\ \sin t & 0 & \cos t \end{pmatrix},$$

$$g_3(t) = \begin{pmatrix} \cos t & -\sin t & 0 \\ \sin t & \cos t & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

For these $g_i(t),\ i = 1, 2, 3$ we get the following tangent matrices (4):

$$e_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad e_2 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

$$e_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Matrices $A_i^{(l)}$ (5) that correspond to representations $T_{g_i(t)}^{(l)}$ are (Gelfand *et al.* (1967)):

$$A_i^{(l)} = (A_i^l)_{mn}, \quad l = 0, 1, \ldots; \ m, n = -l, -l+1, \ldots, 0, \ldots, l-1, l,$$

$$(A_1^l)_{mn} = (A_1^l)_{nm}, \quad (A_1^l)_{mn} = -\tfrac{1}{2} i(\omega_n \delta_{m+1,n} + \omega_m \delta_{m-1,n}),$$

$$(A_2^l)_{mn} = -(A_2^l)_{nm}, \quad (A_2^l)_{mn} = \tfrac{1}{2}(\omega_n \delta_{m+1,n} - \omega_m \delta_{m-1,n}),$$
$$(A_3^l)_{mn} = -im\delta_{mn},$$

where $\omega_m = \sqrt{(l+m)(l-m+1)}$.

THEOREM 2 *By choosing the Lie algebra basis, the normal distribution on* SO(3) *can be reduced to canonical form with three different parameters.*

Proof Let us denote e_1, e_2, e_3 the Lie algebra basis of the SO(3) group. Moreover, let $a_{ij} = V^{-1}\Lambda V$, where Λ is a diagonal matrix of the third order with elements λ_i and V is an orthogonal matrix. If e_1', e_2', e_3' constitute a proper orthogonal basis corresponding to eigenvalues $\lambda_1, \lambda_2, \lambda_3$ then we have

$$\sum_{i,j=1}^{3} a_{ij}\, e_i\, e_j = \sum_{i=1}^{3} \lambda_i\, e_i'\, e_i'. \tag{10}$$

Because of the theorem by Dubrovin *et al.* (1984), and the orthogonality of matrix V, we get $[e_1', e_2'] = e_3'$, $[e_2', e_3'] = e_1'$, $[e_3', e_1'] = e_2'$, and $e_i' = Ve_i$. Thus we find that e_1', e_2', e_3' is a Lie algebra basis of SO(3) group. Moreover, the orthogonal matrix $V = (v_{ij})$ corresponds to some rotation g_0 and to that transformation corresponds a transformation of the group $g \to g_0^{-1}g$, $T_g \to T_{g_0^{-1}g}$. Theorem 2 is proved. We remark that parameters a_i $(i = 1, 2, 3)$ correspond to the "center" of the normal distribution.

Consider a normal distribution in canonical form on the SO(3) group with three parameters,

$$\int_{\mathrm{SO}(3)} T_g^{(l)} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} C_l^{mn} T_l^{mn}(g)\mathrm{d}g = \exp\{B_l\}, \tag{11}$$

where $T_g^{(l)}$ are matrix elements of representation T_g, $B_l = \sum_{i=1}^{3} a_{ii}$ $(A_i^{(l)})^2$ are five diagonal matrices

$$B_l = \left(\begin{array}{ccccccccccc}
b_l^{(1)} & 0 & b_l^{(2)} & & & & & & & & \\
0 & b_{l-1}^{(1)} & 0 & b_{l-1}^{(2)} & & & & & & & \\
b_l^{(2)} & 0 & b_{l-2}^{(1)} & 0 & & & & & & & \\
 & \ddots & & \ddots & & \ddots & & & 0 & & \\
 & & & 0 & b_1^{(1)} & 0 & b_1^{(2)} & & & & \\
 & & & b_1^{(2)} & 0 & b_0^{(1)} & 0 & b_1^{(2)} & & & \\
 & & & & b_1^{(2)} & 0 & b_1^{(1)} & 0 & & & \\
 & & 0 & & & \ddots & & \ddots & & \ddots & \\
 & & & & & & & 0 & b_{(l-2)}^{(1)} & 0 & b_l^{(2)} \\
 & & & & & & & b_{(l-1)}^{(2)} & 0 & b_{(l-1)}^{(1)} & 0 \\
 & & & & & & & & b_l^{(2)} & 0 & b_l^{(1)}
\end{array}\right), \tag{12}$$

with the following elements:

$$
\begin{aligned}
b^{(1)}_{l-m} &= -\tfrac{1}{2}((2m+1)l - m^2)(a_{11}+a_{22}) - (l-m)^2 a_{33},\\
&\quad m = 0, 1, \ldots, l,\\
b^{(2)}_{l-m} &= -\tfrac{1}{4}\sqrt{(m+1)(m+2)(2l-m)(2l-m-1)}\;|a_{11}-a_{22}|,\\
&\quad m = 1, \ldots, l,
\end{aligned} \tag{13}
$$

all other elements are zero. In the case $a_{11} = a_{22} = \nu^2$, $a_{33} = \varrho^2$ we obtain the canonical normal distribution with two parameters

$$
\begin{aligned}
f(g) = \sum_{l=0}^{\infty}(2l+1)\exp\{-l(l+1)\nu^2\} &\sum_{m=-l}^{l} \exp\{m^2(\nu^2-\varrho^2)\\
&- im(\alpha+\gamma)\} P_l^{mm}(\cos\beta),
\end{aligned} \tag{14}
$$

where $P_l^{mm}(\cos\beta)$ is a Jacobi polynomial. In particular, when $\nu^2 = \varrho^2 = \varepsilon^2$ we get a circular normal distribution on SO(3),

$$
f(t) = \sum_{l=0}^{\infty}(2l+1)\exp\{-l(l+1)\varepsilon^2\}\frac{\sin(l+1/2)t}{\sin(t/2)}, \tag{15}
$$

where $\cos(t/2) = \cos(\beta/2)\cos((\alpha+\gamma)/2) = \frac{1}{2}(\mathrm{Tr}(g)-1)$. Here the formula for the character of the representation given by Vilenkin (1968) was used:

$$
\frac{\sin(l+1/2)t}{\sin(t/2)} = \sum_{m=-l}^{l} T_l^{mm}(g).
$$

Distribution (15) is similar to one obtained by Roberts and Winch (1984). Savyolova (1984) presented the following approximation formula

$$
f(t) \sim C(\varepsilon)\frac{t/2}{\sin(t/2)}\exp\left\{\frac{-t^2}{4\varepsilon^2}\right\},
$$

$$
C(\varepsilon) = \frac{\pi}{\varepsilon^3}\exp\left\{\frac{\varepsilon^2}{4}\right\}\mathrm{erfc}\left(\frac{\varepsilon}{2}\right) + \frac{1}{\varepsilon^2}, \quad \varepsilon < 0.5, \ t \sim 0.
$$

Note the connection of the circular normal distribution on SO(3) with the ϑ_2-Jacobi function (Korn and Korn (1968))

$$\vartheta_2(v) = 2\sum_{l=0}^{\infty} q^{(l+1/2)^2}\cos(2l+1)\pi v.$$

Make a change of variables $t = 2\pi v$, $q = \exp(-\varepsilon^2)$, then we get

$$f(t) = -\frac{q^{-1/4}}{2\pi\sin(t/2)}\frac{\partial}{\partial v}\vartheta_2(v).$$

In the paper by Khatri and Mardia (1977) the Mises Fisher matrix distribution was proposed. The expression for that distribution written as a series expansion in terms of spherical harmonics and related functions (according to Watson (1983) such distributions are of some practical interest) depending on the orientation distance t (in our notations) is

$$f(t) = \frac{\exp\{S\cos t\}}{I_0(S) - I_1(S)} = \sum_{l=0}^{\infty}\frac{I_l(S) - I_{(l+1)}(S)}{I_0(S) - I_1(S)}\frac{\sin(l+1/2)t}{\sin(t/2)}, \tag{16}$$

here S is parameter. Correspondence between functions (15) and (16) is discussed by Matthies *et al.* (1988). Figure 1 presents the function (15) and (16) for several values of ε and S.

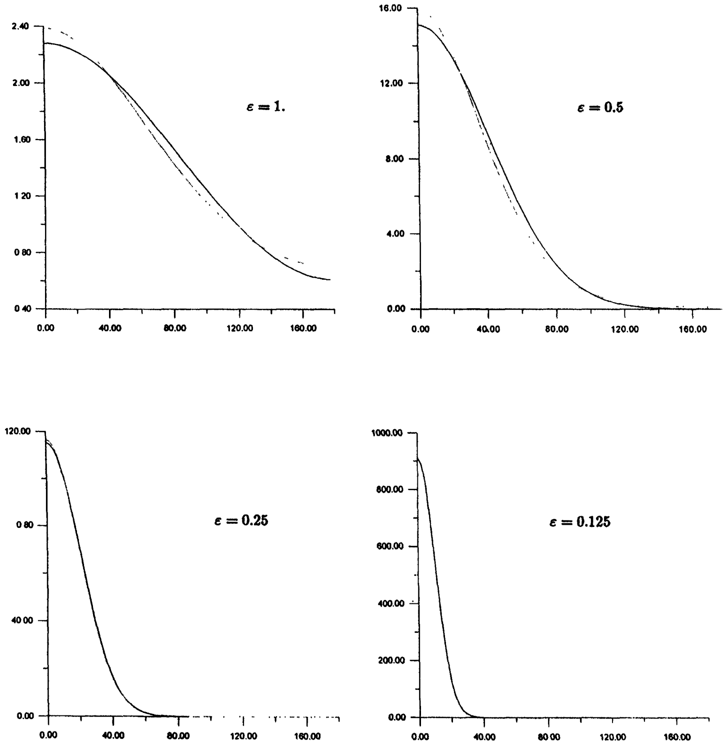
In the case where $a_{ij} = 0$, except $a_{33} = 2\sigma^2$, we get a degenerate normal distribution on SO(3),

$$f(g) = f(\beta) = \frac{1}{\sigma\sqrt{(2\pi)}}\sum_{l=-\infty}^{\infty}\exp\left\{-\frac{(x-2\pi n)^2}{2\sigma^2}\right\}. \tag{17}$$

This function is the same as the normal distribution on the circle SO(2) or the wrapped normal distribution (Mardia (1972)).

THEOREM 3 *Convolution of two circular normal distributions on the* SO(3) *group is again a circular normal distribution.*

Proof Without losing generality it is possible to consider the case when the center of one distribution is e and another is g_0.



$$\max |f^{\text{normal}}(t) - f^{\text{Mizes–Fisher}}(t)| \to \min$$

n	0	1	2	3
$\varepsilon = 2^{-n}$	1	0.5	0.25	0.125
S	0.556	2.19	8.36	32.34

FIGURE 1 Graphics of functions (15) and (16) (dotted). The table at the bottom summarizes parameter values. Values of parameter S were found numerically under the condition.

Convolution on the rotation group is

$$f(g, \varepsilon_1^2) * f(g_0 g, \varepsilon_2^2) = \int_{SO(3)} f(g_1, \varepsilon_1^2) f((g_1)^{-1} g_0 g, \varepsilon_2^2)\, dg_1,$$

where $f(g_0 g, \varepsilon_1^2)$, $f(g, \varepsilon_1^2)$ are functions given in (15) and $g_0 g$ denotes the composite of two rotations. Expanding the circular normal distribution in a series of generalized spherical harmonics we get

$$f(g, \varepsilon_1^2) * f(g_0 g, \varepsilon_2^2) = \int_{\mathrm{SO}(3)} \left(\sum_{l=1}^{\infty} C_l(\varepsilon_1^2) \sum_{m=-l}^{l} T_l^{mm}(g_1) \right) \times \left(\sum_{j=1}^{\infty} C_j(\varepsilon_2^2) \sum_{n=-l}^{l} T_j^{nn}((g_1)^{-1} g_0 g, \varepsilon_2^2) \right) \mathrm{d}g_1,$$

where $C_k(\varepsilon^2) = (2l+1)\exp(-l(l+1)\varepsilon^2)$. Using the addition theorem,

$$T_l^{mn}(g_1 g_2) = \sum_{k=-l}^{l} T_l^{mk}(g_1) T_l^{kn}(g_2),$$

and the orthogonality of the generalized spherical harmonics we find that

$$f(g, \varepsilon_1^2) * f(g_0 g, \varepsilon_2^2) = \sum_{l=1}^{\infty} C_l(\varepsilon_1^2 + \varepsilon_2^2) \sum_{m=-l}^{l} T_l^{mm}(g_0 g) \mathrm{d}g_1$$
$$= f(g_0 g, \varepsilon_1^2 + \varepsilon_2^2).$$

We take into account here that

$$C_l(\varepsilon_1^2) C_l(\varepsilon_2^2) = (2l+1) C_l(\varepsilon_1^2 + \varepsilon_2^2).$$

If we have two arbitrary rotations g_1 and g_2, then because of the invariance of integration on the group we have the proof of the theorem.

Consider examples of fulfilling the conditions of the central limit theorem for the rotation group SO(3) when convergence $f_n^{*n}(g) \to f(g)$ takes place in norms $L_2(\mathrm{SO}(3))$ and $C(\mathrm{SO}(3))$ as $n \to \infty$.

Example 1 Let $f_n(g)$ be the circular normal distribution (15) with parameter ε_n^2. Consider rotations around the OZ axis, or

$$g_3(t) = \begin{pmatrix} \cos t & -\sin t & 0 \\ \sin t & \cos t & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

In this case one can find that

$$g_n = \int_{SO(3)} g\, \mathrm{d}f_n(g) = \begin{pmatrix} 1-3n\varepsilon_n^2 & 0 & 0 \\ 0 & 1-3n\varepsilon_n^2 & 2 \\ 0 & 0 & 1 \end{pmatrix},$$

$$n(e-g_n) = \begin{pmatrix} 3n\varepsilon_n^2 & 0 & 0 \\ 0 & 3n\varepsilon_n^2 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Here e is the identity matrix corresponding to the rotation $g = \{0,0,0\}$. From Theorem 1 under the condition that $n\,\varepsilon_n^2 \leq C = \text{const}$, we get that parameters of the limit normal distribution, $f(g) = \lim_{n\to\infty} f_n^{*n}(g)$, are the following: $a_{ij} = 0$, except $a_{33} = 2\,\sigma^2$. Therefore the limit distribution is a normal distribution of rotations around the OZ axis or the normal distribution on the circle.

Example 2 Let $f_n(g)$ be the normal distribution (14) of canonical form with two parameters. In that case $g_n = (g_{ij}^n)$, where $g_{11}^n = g_{22}^n = \exp\{-\nu_n^2 - \varrho_n^2\}$, $g_{33}^n = \exp\{-2\nu_n^2\}$, and all other $g_{ij}^n = 0$. From here we get that if $n\nu_n^2 \to \nu_2$, $n\varrho_n^2 \to \varrho^2$, then the limit distribution will be normal with two parameters. In particular, when $\nu^2 = \varrho^2 = \varepsilon^2$ we get the circular normal distribution (15).

THEOREM 4 *The convergence* $f_k^{*k} \to f(g)$ *as* $k \to \infty$ *where* $f(g)$ *is the normal distribution on* SO(3) *is assured if and only if for eigenvalues of matrices of Fourier coefficients of distributions* $f_k(g)$ *hold:*

$$\lim_{k\to\infty} \lambda_i^k = \exp\tilde{\lambda}_i,$$

where $\tilde{\lambda}_i$ *are some real constants.*

Proof If the distribution $f_k(g)$ corresponds to a matrix of Fourier coefficients $C_l = c_l^{mn}, m, n = 0, \pm 1, \ldots, \pm l$; $l = 0, 1, \ldots$ then the distribution $f_k^{*k}(g)$ corresponds to the kth power of matrix C_l, or matrix $C_l^k = (C_l^{mn})^k$. If the matrices C^l are hermitian, then $C_l = (U_l)^{-1} \Lambda_l U_l$, where U_l is an orthogonal matrix, Λ_l is diagonal with elements λ_i. For C_l^k we get $C_l^k = (U_l)^{-1}(\Lambda_l)^k U_l$. From (6) we find

$$\lim_{n\to\infty} \int_{SO(3)} T_g^{(l)} f_n^{*n}\, \mathrm{d}g = \int_{SO(3)} T_g^{(l)} f(g) \mathrm{d}g = \exp(B_l).$$

Since matrix B_l is hermitian, an analogous representation is valid: $B_l = (U_l)^{-1}\tilde{\Lambda}_l U_l$. Therefore $\exp(B_l) = (U_l)^{-1}\exp(\tilde{\Lambda}_l)U_l = \lim_{n\to\infty} (U_l)^{-1}\Lambda_l^k U_l$ and this establishes the result.

3 NORMAL DISTRIBUTION AS A FUNDAMENTAL SOLUTION OF THE DIFFUSION EQUATION

Consider the equation

$$\frac{1}{\sin^{n-2}\beta}\frac{\partial}{\partial\beta}\left(\sin^{n-2}\frac{\partial f(\beta,t)}{\partial\beta}\right) = \frac{1}{R}\frac{\partial f(\beta,t)}{\partial t}, \tag{18}$$

where $\beta \in [0,\pi]$, $R > 0, t \geq 0, n \geq 2$.

Definition The fundamental solution of Eq. (18), $f_{n-1}(\beta,t) \equiv F_{n-1}(u,t)$ where $u \equiv \cos\beta$, is one that possesses the following properties:

$$s_{n-1}\int_0^{\pi} f_{n-1}(\beta,t)\sin^{n-2}\beta \,\mathrm{d}\beta = 1, \quad f_{n-1}(\beta,0) = \frac{\delta(\beta)}{s_{n-1}\sin^{n-2}\beta},$$
$$s_{n-1} = \frac{2\pi^{n/2}}{\Gamma(n/2)}. \tag{19}$$

The fundamental solution of Eq. (18) is the following:

$$\begin{aligned} f_{n-1}(\beta,t) &\equiv F_{n-1}(u,t) \\ &= \frac{1}{s_{n-1}2p}\sum_{l=0}^{\infty}(2l+2p)\exp\{-l(l+2p)Rt\}C_l^p(u), \end{aligned} \tag{20}$$

where $p = (n-2)/2 > 0$ and $C_l^p(u)$ are Gegenbauer polynomials.

From Eq. (18) at $n=2$ we get

$$\begin{aligned} F_1(u,t) &= \frac{1}{2\pi}\sum_{l=0}^{\infty} 2l\exp\{-l^2Rt\}C_l^0(u) \\ &= \frac{1}{\pi}\sum_{l=0}^{\infty} 2l\exp\{-l^2Rt\}\cos l\beta. \end{aligned} \tag{21}$$

For the normal distribution on the circle SO(2). Note that the function (19) was obtained in (Parthasarathy (1967)) from the central limit theorem on the circle SO(2). We obtained it from the central limit theorem on SO(3) as the degenerate case (17).

From Eq. (18) at $n=3$ we get

$$F_2(u,t)=\frac{1}{4\pi}\sum_{l=0}^{\infty}(2l+1)\exp\{-l(l+1)Rt\}P_l(u), \tag{22}$$

for the normal distribution on the sphere S^2 in $\mathbf{R}^3$.

At $n=4$ from Eq. (18) we get the normal distribution on the sphere S^3 in $\mathbf{R}^4$

$$F_3(u,t)=\frac{1}{4\pi^2}\sum_{l=0}^{\infty}(2l+1)\exp\{-l(l+1)Rt\}\frac{\sin(l+1)\beta}{\sin\beta}. \tag{23}$$

At the transition from SU(2) to SO(3) we take in Eq. (18) only l even and obtain the normal distribution on SO(3):

$$\widetilde{F}_3(u,t)=\frac{1}{2\pi^2}\sum_{l=0}^{\infty}(2l+1)\exp\{-l(l+1)Rt\}\frac{\sin(l+1)\tilde{\beta}}{\sin\tilde{\beta}}, \tag{24}$$

where $\tilde{\beta}=2\beta$. We obtained (23) from the definition of normal distribution and the central limit theorem on SO(3) in (15).

THEOREM 5 *The fundamental solution of Eq.* (18), $f_{n-1}(\beta,t)$ *is nonnegative and infinitely differentiable at* $t>0$.

Proof To prove the differentiability of the function (18) it is possible to use the formula for the derivative of a Gegenbauer polynomial (Vilenkin (1968)). As a result we get

$$\frac{\partial^k F_{n-1}(u,t)}{\partial u^k}=\frac{2^k\Gamma(p+k)}{s_{n-1}\,p}\sum_{l=0}^{\infty}(l+p)\exp\{-l(l+1)Rt\}C_{l-k}^{p+k}(u). \tag{25}$$

Therefore function $F_{n-1}(u,t)$ in (18) is differentiable at $k=1,2,\ldots$, $t>0$. To prove that the function $F_{n-1}(u,t)\geq 0$ at $t>0$, $\beta\in[0,\pi]$ suppose the opposite. Let $F_{n-1}(u,t)<0$ at $t=\bar{t}>0$. Denote $\min_u F_{n-1}(u,t)=\alpha<0$ at point $\beta=\bar{\beta}$. (Treat the maximum of the function analogously.) Hence, from Eq. (18), $\partial F_{n-1}(u,t)/\partial t|_{\beta=\bar{\beta}} \geq 0$. Since $F_{n-1}(u,t)|_{t=0} = 0$, $u \neq 0, \partial F_{n-1}(u,t)/\partial t|_{\beta=\bar{\beta}} \geq 0$ then $F_{n-1}\ (u,t)$ $|_{\beta=\bar{\beta}} \leq 0$ is impossible. Analogously at $\bar{\beta} = \pi, F_{n-1}\ (u,t)|_{\beta=\bar{\beta}} \leq 0$ is impossible, since from initial condition, $F_{n-1}(-1,0) = 0$. As $t \to 0+$, $F_{n-1}(-1,0) \geq (s_{n-1})[1 - 2(l+p)Rt] > 0$. Further, the inequality holds because $\partial F_{n-1}(u,t)/\partial t|_{\beta=\bar{\beta}} \geq 0$. The theorem is proved.

4 NORMAL DISTRIBUTION ON S^2 AND ITS PROPERTIES

The unified view on the directional statistics is given by Jupp and Mardia (1989). We suggest a different approach to the distributions on the two-dimensional sphere.

The unit sphere S^2 in $\mathbf{R}^3$ can be identified with the space of adjacent classes $\{uh\}$, $u \in \mathrm{SU}(2)$, $h \in \Omega$, where

$$h = \begin{pmatrix} \exp\{it/2\} & 0 \\ 0 & \exp\{it/2\} \end{pmatrix}.$$

To each adjacent class $u\,\Omega$ corresponds a point $\xi \in \mathrm{S}^2$, $\{-\pi/2 = \alpha,\ \beta\}$, $u = u\ (\alpha, \beta, \gamma)$. Therefore functions $f(\xi)$, $\xi \in S^2$ can be obtained from functions $f(u)$, $u \in \mathrm{SU}(2)$, by maintaining the following condition $f(hu) \equiv f(u)$, $h \in \Omega$.

Thus, normal distribution $f(\xi)$ on S^2 can be obtained from Eq. (6) at $a_{ij} = 0$ when $i = 3$ or $j = 3$, since the infinitesimal operator of representation A_3 corresponds to the subgroup Ω as follows:

$$\begin{aligned} f(\xi)\mathrm{d}\xi &= \frac{1}{8\pi^2}\int_0^{2\pi} \mathrm{d}\gamma\, f(\alpha,\beta,\gamma)\sin\beta\,\mathrm{d}\beta\,\mathrm{d}\alpha \\ &= \frac{1}{4\pi}\sum_{l=0}^{\infty}\sum_{m=-l}^{l} C_l^{m0} T_l^{m0}(g)\sin\beta\,\mathrm{d}\,\beta\,\mathrm{d}\alpha. \end{aligned} \tag{26}$$

In particular, at $a_{11} = a_{22} = \nu^2$ and $a_{12} = a_{21} = 0$ we get from (6) at $a_{33} = a_{13} = a_{31} = 0$, $a + 1 = l_2 = a_3 = 0$, the circular normal distribution on S^2,

$$f(\beta) = \sum_{l=1}^{\infty}(2l+1)\exp\{-l(l+1)a^2\}P_l(\cos\beta), \tag{27}$$

where $P_l(\cos\beta)$ are Legendre polynomials.

We remark that the circular normal distribution on S^2 (26) was obtained by Perrin (1972) from a study of Brownian motion. We suggest the following definition of a normal distribution on S^2.

DEFINITION The normal distribution S^2 is defined by (26) for $f(g)$ from (26) at $a_{ij}=0$ when $i=0$ or $j=3$. In particular, the circular normal distribution on S^2 can be expressed by (27).

The distribution on the sphere S^2 (27) approximates the well-known Fisher distribution. This is discussed in detail by Watson (1983).

5 COMPUTATION OF THE NORMAL DISTRIBUTION

Computing of the normal distribution on SO(3) is a separate, serious problem. This section presents methods for these computations and some estimates of accuracy in different metrics.

Coefficients of normal distribution at each l create matrix C_l of order $2l+1$ where

$$C_l = \exp\{B_l\}. \tag{28}$$

Explicit expressions for the matrix and its elements are given by (12) and (13).

Since B_l is a symmetric matrix, it can be represented in the form $B_l = (U_l)^{-1}\Lambda U_l$, where U_l is orthogonal, Λ_l is a diagonal and its elements are the eigenvalues of B_l. The expression $\exp(B_l) = (U_l)^{-1}$ $\exp(\Lambda_l)U_l$ is therefore valid. At $l=0$ $(C_0)_{00} = 1$. At $l=1$ one can obtain

$$\begin{aligned}
&\sum_{m=-1}^{1}\sum_{n=-1}^{1} C_l^{mn} T_l^{mn}(g) \\
&\quad = \frac{3}{2}\,\{2e^{-(a_{11}+a_{22})}\cos\beta \\
&\qquad + (e^{-(a_{11}+a_{33})} + e^{-(a_{22}+a_{33})})\cos(\alpha+\gamma)(1+\cos\beta) \\
&\qquad - (e^{-(a_{11}+a_{33})} - e^{-(a_{22}+a_{33})})\cos(\alpha-\gamma)(1-\cos\beta)\}.
\end{aligned}$$

We have found formulae for $l=2$ and 3, but it seems possible to reach arbitrary accuracy calculating normal distribution with three different parameters only by numerical computations. We give an algorithm calculating the matrix $\exp B_l$ and estimates of the spectrum of matrix B_l.

Decomposition of the matrix B_l for commutative parts The property of matrix exponents:

$$e^{A+B} = e^A e^B = e^B e^A \tag{29}$$

is valid if $AB = BA$. We imply further that l is even. (That is only for simplification of the notes. For l odd everything is almost the same.) Matrix B_l can be represented in the form

$$B_l = R_l + S_l. \tag{30}$$

Matrix R_l has as the only nonzero elements $(R_l)_{mn}$ $(m, n = -l, -l+1, \ldots, 0, 1, \ldots, l)$ such that m and n are both even; matrix S_l has the only nonzero elements with m and n both odd. Because of this construction

$$R_l S_l = S_l R_l.$$

Therefore, the matrix of coefficients of the canonical normal distribution is

$$C_l = \exp B_l = \exp R_l \exp S_l = \exp S_l \exp R_l.$$

We remark that the coefficients $(C_l)_{mn}$ with both m and n even depend only on R_l and with both m and n odd depend only on S_l. Moreover, $(C_l)_{mn} = 0$ when $m + n$ is odd.

If B_l is symmetric about the origin then the matrix $C_l = \exp B_l$ is symmetric about the origin, too. For the matrix $C_l = \exp B_l$ the following symmetry relationships hold:

$$(C_l)_{mn} = (C_l)_{nm} = (C_l)_{2l+1-m,\, 2l+1-n} = (C_l)_{2l+1-n,\, 2l+1-m}.$$

It is possible to see this by direct computation of the product of arbitrary symmetrical matrices and the following formula for a matrix exponent:

$$\exp D = E + \frac{D}{1!} + \frac{D^2}{2!} + \cdots,$$

where D is an arbitrary matrix.

It can be seen that the matrices R_l and S_l have a lot of zeros. By means of elementary transformations $(Q_l)_{mn}$ of transformation of lines and columns they can be evaluated to more convenient form for computation. Matrix $(Q_l)_{mn}$ is the following:

$$(Q_l)_{mn} = E - (E_l)_{mm} - (E_l)_{nn} + (E_l)_{mn} + (E_l)_{nm},$$

where E_l is an identity matrix of order $2l+1$, $(E_l)_{ij}$ is a square matrix of order $2l+1$, with ones on the intersection of ith line and jth column and all other elements zeros. If A_l is some arbitrary matrix then $(Q_l)_{mn}A_l$ can be obtained from A_l by means of transposition of the mth and nth lines, $A_l(Q_l)_{mn}$ can be obtained from A_l by means of transposition of the mth and nth columns. Moreover, $(Q_l)_{mn}(Q_l)_{mn} = E_l$.

Introduce the matrix $U_l = (Q_l)_{l+1,2l+1}\ldots(Q_l)_{k+1,2k+1}\ldots(Q_l)_{23}$ $(k = 1,\ldots,l)$ then the matrix $'R_l = U_lR_l(U_l)_{-1}$ will be

$$'R_l = \begin{pmatrix} r_l & \vdots & 0 \\ \ldots & \ldots & \ldots \\ 0 & \vdots & 0 \end{pmatrix},$$

where r_l is a tridiagonal symmetric matrix. Matrix $'R_l$ has the order $2l+1$ and the matrix r_l has order $l+1$.

Analogously for the matrix S_l we can construct $'S_l = V_lS_l(V_l)_{-1}$ where $V_l = (Q_l)_{l,2l}\ldots(Q_l)_{k,2k}\ldots(Q_l)_{12}$ $(k = 1,\ldots,l)$. Matrix $'S_l$ is

$$'S_l = \begin{pmatrix} s_l & \vdots & 0 \\ \ldots & \ldots & \ldots \\ 0 & \vdots & 0 \end{pmatrix},$$

where s_l is a tridiagonal symmetric matrix. Matrix $'S_l$ has the order $2l+1$ and the matrix s_l has order l. Because of the orthogonality of the matrices $(Q_l)_{mn}$ it is possible to write

$$\exp B_l = (U_l)_{-1} \exp('R_l)U_l(V_l)_{-1} \exp('S_l)V_l. \tag{31}$$

If u_l is the orthogonal matrix of order $l+1$ such that $u_lr_l(u_l)^{-1} = \lambda_l$, where λ_l is the diagonal matrix of order $l+1$ then:

$$'R_l = \begin{pmatrix} u_l^{-1} & \vdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \vdots & E_l \end{pmatrix} \begin{pmatrix} \lambda_l & \vdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \vdots & 0 \end{pmatrix} \begin{pmatrix} u_l & \vdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \vdots & E_l \end{pmatrix}.$$

Therefore we have

$$\exp('R_l) = \begin{pmatrix} u_l^{-1} & \vdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \vdots & E_l \end{pmatrix} \begin{pmatrix} \exp(\lambda_l) & \vdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \vdots & E_l \end{pmatrix} \begin{pmatrix} u_l & \vdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \vdots & E_l \end{pmatrix}$$

$$= \begin{pmatrix} \exp(r_l) & \vdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \vdots & E_l \end{pmatrix}.$$

Analogously we can get

$$\exp('S_l) = \begin{pmatrix} \exp(s_l) & \vdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \vdots & E_l \end{pmatrix}.$$

Thus we prove Theorem 6.

THEOREM 6 *Computation of* $\exp B_l$ *where matrix* B_l (12) *with matrix elements* (13) *has five diagonals of order* $2l+1$ *is equivalent to computation of* $\exp r_l$ *and* $\exp s_l$ *where the matrices* r_l *and* s_l *have orders* $l+1$ *and* l *respectively and they are symmetrical tridiagonal.*

Estimates and asymptotics with $l \to \infty$ *of spectrum* B_l *and matrix elements of* $\exp B_l$ Here we will give estimates of Jacobi's matrices spectra as a function of normal distribution parameters.

LEMMA 1 *For spectrum of matrices* r_l*, it is*

$$X_r \le \lambda_i \le Y_r \quad (i = 1, 2, \ldots, l+1),$$

where for l even,

$$X_r = \begin{cases} b_0^{(1)} - 2|b_2^{(2)}| & \text{when } a_{11} + a_{22} \geq 2a_{33}, \\ b_l^{(1)} - 2|b_2^{(2)}| & \text{when } a_{11} + a_{22} < 2a_{33}, \end{cases}$$

$$Y_r = \begin{cases} b_l^{(1)} + 2|b_2^{(2)}| & \text{when } a_{11} + a_{22} \geq 2a_{33}, \\ b_0^{(1)} + 2|b_2^{(2)}| & \text{when } a_{11} + a_{22} < 2a_{33}, \end{cases}$$

and for l odd,

$$X_r = \begin{cases} b_0^{(1)} - 2|b_2^{(2)}| & \text{when } a_{11} + a_{22} \geq 2a_{33}, \\ b_{l-1}^{(1)} - 2|b_2^{(2)}| & \text{when } a_{11} + a_{22} < 2a_{33}, \end{cases}$$

$$Y_r = \begin{cases} b_{l-1}^{(1)} - 2|b_2^{(2)}| & \text{when } a_{11} + a_{22} \geq 2a_{33}, \\ b_0^{(1)} - 2|b_2^{(2)}| & \text{when } a_{11} + a_{22} < 2a_{33}, \end{cases}$$

where

$$b_0^{(1)} = -\tfrac{1}{2}l(l+1)(a_{11} + a_{22}), \quad b_l^{(1)} = -\tfrac{1}{2}l(a_{11} + a_{22}) - l^2 a_{33},$$

$$b_{l-1}^{(1)} = -\tfrac{1}{2}(3l-1)(a_{11} + a_{22}) - (l-1)^2 a_{33},$$

$$2|b_2^{(2)}| = \sqrt{l(l+1)(l^2-1)}|a_{11} - a_{22}|.$$

Proof For symmetrical tridiagonal matrix the following Godunov (1977) estimates are valid:

$$X_r \leq \lambda_i \leq Y_r,$$

where (in our notation)

$$X_r = \max_{k=1,\dots,l/2-2} x_k, \quad x_k = \begin{cases} b_l^{(1)} - |b_l^{(2)}|, \\ b_{l-2k}^{(1)} - (|b_{l-2k}^{(2)}| + |b_{l-2k-2}^{(2)}|), \\ b_0^{(1)} - 2|b_2^{(2)}|, \end{cases}$$

$$Y_r = \max_{k=1,\dots,l/2-2} y_k, \quad y_k = \begin{cases} b_l^{(1)} + |b_l^{(2)}|, \\ b_{l-2k}^{(1)} + (|b_{l-2k}^{(2)}| + |b_{l-2k-2}^{(2)}|), \\ b_0^{(1)} + 2|b_2^{(2)}|. \end{cases}$$

Index r means that estimations are for matrices r_l. Matrix elements are monotonic. We get our lemma from the above-mentioned estimates and the monotonicity of the elements.

LEMMA 2 *For spectrum of matrices s_l, it is*

$$X_s \leq \lambda_i \leq Y_s \quad (i = 1,2,\ldots,l),$$

where for l even,

$$X_r = \begin{cases} b_1^{(1)} - (|b_1^{(2)}| + |b_3^{(2)}|) & \textit{when } a_{11} + a_{22} \geq 2a_{33}, \\ b_{l-1}^{(1)} - (|b_1^{(2)}| + |b_3^{(2)}|) & \textit{when } a_{11} + a_{22} < 2a_{33}, \end{cases}$$

$$Y_r = \begin{cases} b_{l-1}^{(1)} + (|b_1^{(2)}| + |b_3^{(2)}|) & \textit{when } a_{11} + a_{22} \geq 2a_{33}, \\ b_1^{(1)} + (|b_1^{(2)}| + |b_3^{(2)}|) & \textit{when } a_{11} + a_{22} < 2a_{33}, \end{cases}$$

and for l odd,

$$X_r = \begin{cases} b_1^{(1)} - (|b_1^{(2)}| + |b_3^{(2)}|) & \textit{when } a_{11} + a_{22} \geq 2a_{33}, \\ b_l^{(1)} - (|b_1^{(2)}| + |b_3^{(2)}|) & \textit{when } a_{11} + a_{22} < 2a_{33}, \end{cases}$$

$$Y_r = \begin{cases} b_l^{(1)} + (|b_1^{(2)}| + |b_3^{(2)}|) & \textit{when } a_{11} + a_{22} \geq 2a_{33}, \\ b_1^{(1)} + (|b_1^{(2)}| + |b_3^{(2)}|) & \textit{when } a_{11} + a_{22} < 2a_{33}, \end{cases}$$

where

$$\begin{aligned} b_1^{(1)} &= -\tfrac{1}{2}(l^2 + l - 1)(a_{11} + a_{22}), \\ b_l^{(1)} &= -\tfrac{1}{2}l(a_{11} + a_{22}) - l^2 a_{33}, \\ b_{l-1}^{(1)} &= -\tfrac{1}{2}(3l - 1)(a_{11} + a_{22}) - (l-1)^2 a_{33}, \\ (|b_1^{(2)}| + |b_3^{(2)}|) &= (l(l+1) + \sqrt{(l-1)(l+3)(l^2-4)})|a_{11} - a_{22}|. \end{aligned}$$

Proof of the lemma is analogous to that of Lemma 1.

We remark that matrix B_l is singular when two parameters out of three (a_{11}, a_{22}, a_{33}) are equal to zero. In all other cases B_l is nonsingular. Matrix r_l is singular when B_l is singular. Matrix s_l is singular only in the case $a_{11} = a_{22} = a_{33} = 0$. It is interesting that in the nonsingular case $\det(B_l) = \det(r_l)\det(s_l)$.

THEOREM 7 *The set of eigenvalues of matrix B_l is the union of the sets of eigenvalues of matrices r_l and s_l.*

Proof 1. Consider the vector space V_l $\dim V_l = 2l + 1$. Matrix B_l can be considered as the matrix of the operator $\mathcal{B}_l$ and because of the nonsingularity of B_l, $\operatorname{Ker} \mathcal{B}_l = 0$. In V_l there exist the basis $e_i = (0, \dots, 1, \dots, 0)$ $i = -l, \dots, l$. Divide V_l into two subspaces V_l^* and V_l^{**} with basis e_{2k} $k = -l/2, -l/2 + 1, \dots, l/2$ and e_{2p+1} $p = -l/2, -l/2 + 1, \dots, l/2 - 1$. One can see that the operator $\mathcal{R}_l$ (with matrix R_l) reflects V_l^* on itself and $\mathcal{S}_l$ (with matrix S_l) reflects V_l^{**} on itself and

$$\mathcal{R}_l V_l^* = V_l^*, \quad \mathcal{S}_l V_l^* = 0,$$

$$\mathcal{R}_l V_l^{**} = 0, \quad \mathcal{S}_l V_l^{**} = V_l^{**}.$$

We can ensure that this property holds by looking at the efficiency of operators $\mathcal{R}_l(\mathcal{S}_l)$ on the basis e_i.

2. Each eigenvector of matrix $R_l(S_l)$ that correspond to a nonzero eigenvalue is at the same time an eigenvector of matrix B_l with the same eigenvalue. Let $R_l x_l = \lambda_l x_l$, then

$$B_l x_l = (R_l + S_l)x_l = R_l x_l + S_l x_l = R_l x_l = \lambda_l x_l.$$

3. Each eigenvalue of matrix $R_l(S_l)$ and eigenvalues of $'R_l('S_l)$ are the same. Eigenvalues of R_l are obtained from $\det(R_l - \lambda_l E_l = 0$, but R_l and $'R_l$ are connected with each other by $R_l = U_l\, 'R_l(U_l)^{-1}$, so we have

$$\begin{aligned}\det(R_l - \lambda_l E_l) &= \det(U_l\, 'R_l(U_l)^{-1} - \lambda_l E_l) \\ &= \det(U_l)\det('R_l - \lambda_l E_l)\det(U_l^{-1}) = \det('R_l - \lambda_l E_l).\end{aligned}$$

Nonzero eigenvalues of matrix $'R_l('S_l)$ are identical with nonzero eigenvalues of matrix $r_l(s_l)$. This follows from the block structure of the matrices.

COROLLARY 1 *Estimates of the eigenvalues of B_l follow from Theorem* 2 *and Lemmas* 1 *and* 2:

$$\lambda_i \le W_l = \begin{cases} b_l^{(1)} + 2|b_2^{(2)}|, & l \textit{ even when } a_{11} + a_{22} \ge 2a_{33}, \\ b_l^{(1)} + (|b_1^{(2)}| + |b_3^{(2)}|), & l \textit{ odd when } a_{11} + a_{22} \ge 2a_{33}, \\ b_0^{(1)} + 2|b_2^{(2)}|, & \textit{when } a_{11} + a_{22} < 2a_{33}. \end{cases}$$

When $l \to \infty$ we have

$$W_l = \begin{cases} (-l^2 a_{33} - 1/2l(a_{11} + a_{22}) + 1/2l(l+1)|a_{11} - a_{22}|)(1 + O(l^{-1})), \\ (-1/2l(l+1)(a_{11} + a_{22}) + 1/2l^2|a_{11} - a_{22}|)(1 + O(l^{-1})), \\ (-l^2 a_{33} - 1/2l(a_{11} + a_{22}) + 1/2l(l+1)|a_{11} - a_{22}|)(1 + O(l^{-1})). \end{cases}$$

COROLLARY 2 *As far as the spectral norm of matrix is equal to absolute value of the maximal eigenvalue, then*

$$\|C_l\| = \|\exp B_l\| \le \exp W_l.$$

From here we can get the following estimates for elements of matrix C_l:

$$|C_l^{mn}| \le \exp W_l.$$

It is known that the square of a matrix's eucledian norm is equal to the sum of singular values, or

$$C_l = \exp\{B_l\}. \tag{32}$$

$$\|C_l\|^2 \le (2l+1)\exp 2W_l. \tag{33}$$

Remark 1 All estimates become exact in the circular case.

Remark 2 Here we have considered band matrices, with only three diagonal nonzero. However, all results, almost without any changes, can be transferred to band matrices with any amount of diagonals with only the constraint that they must have zero elements with odd sum of indices.

Estimates in the circular case In computations using the circular normal distribution on SO(3) and S^2, (15) and (27), a question arises about the number of series terms required to compute these functions to a given accuracy. Expressions for the remainders of (15) and (27) are given below as functions of the parameter ε in two metrics.

The remainders of (15) in $L_2(\mathrm{SO}(3))$ norm are

$$\|\delta F(t)\|_{L_2(\mathrm{SO}(3))} = \pi^{-1}\int_0^{2\pi} |\delta f(t)|^2 \sin^2\frac{t}{2}\mathrm{d}t$$
$$= \sum_{l=N}^{\infty}(2l+1)^2 \exp(-2l(l+1)\varepsilon^2), \quad F(t) = f(t)\sin\frac{t}{2}, \tag{34}$$

where

$$f(t) = \sum_{l=N}^{\infty}(2l+1)\exp(-l(l+1)\varepsilon^2)\frac{\sin(l+1/2)t}{\sin(t/2)}.$$

We have the following estimate of expression (34):

$$\|\delta F(t)\|_{L_2(\mathrm{SO}(3))} = (2N+1)^2 \exp(-2N(N+1)\varepsilon^2)$$
$$+\frac{\sqrt{2\pi}}{4\varepsilon^2}\exp(\varepsilon^2/2)\,\mathrm{erfc}(\sqrt{2}\varepsilon(N+1/2)).$$

Analogously for function (27) we get the estimate of the remainder,

$$\|\delta f_2(t)\|_{L_2(S^2)} = \sum_{l=N}^{\infty}(2l+1)^2 \exp(-2l(l+1)\varepsilon^2)$$
$$= (2N+1)^2 \exp(-2N(N+1)\varepsilon^2)$$
$$+\frac{\sqrt{2\pi}}{4\varepsilon^2}\exp(\varepsilon^2/4)\mathrm{erfc}(\sqrt{2}\varepsilon(N+1/2)),$$

where

$$f_2(g) = \sum_{l=N}^{\infty}(2l+1)\exp(-l(l+1)\varepsilon^2)P_l(\cos t).$$

The estimate of the remainder of the circular normal distribution in a contiguous metric is

$$\begin{aligned}\|\delta F(t)\|_{C(\mathrm{SO}(3))} &= |\max \delta f(t)\sin^2\frac{t}{2}| \\ &= \sum_{l=N}^{\infty}(2l+1)\exp(-l(l+1)\varepsilon^2) \\ &= \frac{1}{\varepsilon^2}\exp(-N(N+1)\varepsilon^2). \qquad (35)\end{aligned}$$

Let η be the ratio after the summation over all terms to the remainder after summation over the first N terms

$$\eta = \left\{\sum_{l=N}^{\infty}(2l+1)\exp(-l(l+1)\varepsilon^2)\right\}\Big/\left\{\sum_{l=0}^{\infty}(2l+1)\exp(-l(l+1)\varepsilon^2)\right\}$$

Then the following inequality holds:

$$\eta \geq \exp(-N(N+1)\varepsilon^2).$$

From this we get

$$N \geq \sqrt{1/4 - \varepsilon^{-1}\ln\eta} - 1/2.$$

Analogous to expression (34) for the function (26) we get the estimate of the remainder in a contiguous metric:

$$\begin{aligned}\|\delta f_2(t)\|_{C(S^2)} &= \sum_{l=N}^{\infty}(2l+1)^2\exp(-2l(l+1)\varepsilon^2) \\ &= \frac{N+1/2}{\varepsilon}\exp(-N(N+1)\varepsilon^2) \\ &\quad + \frac{\sqrt{\pi}}{\varepsilon^2}\exp(\varepsilon^2/4)\mathrm{erfc}(\varepsilon(N+1/2)).\end{aligned}$$

Given expressions for estimating of the remainders of the circular normal distribution on the rotation group in L_2 metric be obtained from previous estimators (31).

In the end of this section we present analytic expressions that approximate circular normal distribution on the group and sphere. Bunge (1982) suggested the following normal distribution on SO(3):

$$f(g) = f(t) = C \exp\left\{-\frac{t^2}{\pi^2 \varepsilon^2}\right\}, \tag{36}$$

where C is a constant that can be defined from (36), $\cos t = \frac{1}{2}(\mathrm{Tr}(g) - 1)$ and g is a rotation matrix. Matthies *et al.* (1988) showed that (35) and (15) approximate each other for small values of the parameter ε.

6 CONCLUSION

We have considered the definition of the normal distributions on the nonabelian SO(3) group, its projection to the sphere S^2, methods of computation, and some properties and application to a texture analysis problem. These results can be generalized to groups SO(n) and spheres S^{n-1}, $n \geq 4$.

It was shown that the circular normal distribution (15) satisfies Parthasarathy's central limit theorem, is a solution of the diffusion equation and that the convolution of such distributions is again a distribution of the same type.

However, many questions require further study. A normal but not circular distribution was studied inadequately. So far as this distribution can be obtained only numerically, it would be useful to have simple approximation formulas for computations. A theorem about the convolution of two normal distributions with arbitrary parameters is not obtained and it is not clear if it has a place in that case. There is no central limit theorem for the sphere S^2 for the Perrin distribution.

APPENDIX: APPLICATION OF NORMAL DISTRIBUTION TO THE SOLUTION OF A TEXTURE ANALYSIS PROBLEM

Preliminary notes Texture is a collection of monocrystalline orientations that compose the polycrystalline sample. It has an essential influence on behavior and properties of a polycrystal. This is the reason why a full quantitative description of texture and estimations of properties of samples with different texture are important.

Consider a polycrystalline sample. A coordinate system K_A is connected with the sample; a coordinate system K_B is connected with a crystallite in that sample. Orientation of a crystallite relative to the polycrystal can be described with the rotation $g : K_B \xrightarrow{g} K_A$. A quantitatively more detailed description of texture is possible through an orientation distribution function $f(g)$. It is important to note that "orientation distribution function" is a common but not precise term. Under an orientation distribution function one assumes density of orientation distribution or orientation density function. Let V volume of sample and $\mathrm{d}V(g)$ be a volume of monocrystals in the sample with orientation g.

DEFINITION Orientation distribution function is the function $f(g)$, $g \in \mathrm{SO}(3)$, that satisfies condition

$$\frac{\mathrm{d}V(g)}{V} = f(g)\mathrm{d}g,$$

where $g = \{\alpha, \beta, \gamma\}$, $0 \leq \alpha, \gamma < 2\pi$, $0 \leq \beta \leq \pi$ are Euler angles of rotation and $\mathrm{d}g = \mathrm{d}\alpha \sin\beta \,\mathrm{d}\beta \,\mathrm{d}\gamma$ is an invariant measure on SO(3). Volume of sample is supposed to be equal to the joint volume of all monocrystals and only the orientation of crystallites rather than their spatial position is taken into account. It follows from the definition that $f(g)$ is nonnegative and, moreover,

$$\int_{\mathrm{SO}(3)} f(g)\mathrm{d}g = 1. \tag{37}$$

Because of the symmetry of crystallite for rotations g and $g_{B_j}g$ where $g_{B_j} \in G_B$ is a crystallite symmetry group, the following relation must be fulfilled:

$$f(g) = f(g_{B_j}g), \tag{38}$$

and if there is sample symmetry,

$$f(g) = f(g_{B_j}gg_{A_k}), \tag{39}$$

where $g_{A_k} \in G_A$ is a sample symmetry group. If there is some function $f(g)$, it can be symmetrized as follows to obey properties (38) and (39):

$$f(g) = \frac{1}{N_B} \sum_{j=1}^{N_B} f(g_{B_j} g), \quad f(g) = \frac{1}{N_A N_B} \sum_{j=1}^{N_B} \sum_{k=1}^{N_A} f(g_{B_j} g g_{A_K}).$$

Experiemntal information about the orientation distribution function can be obtained if all sample crystallites volumes and orientations can be measured, but such information can only be obtained with the destruction of the sample and is very expensive. The number of crystallites in a sample is tens of thousands (in large grain samples) to tens of millions (in small grain samples). Another source of information about the orientation distribution function is pole figures, denoted as $P_{\mathbf{h}_i}(\mathbf{y})$ which are projections of the orientation distribution function. These functions are measured in diffraction experiments (X-ray or neutron); for a detailed description see Bunge (1982). If $\mathbf{y}$ is a unit vector that describes some direction in a sample coordinate system and $\mathbf{h}_i$ is a unit vector that describes some direction in a crystallite coordinate system, $\mathrm{d}V(\mathbf{h}_i \| \mathbf{y})$ is a volume of crystallites whose crystallographic direction $\mathbf{h}_i$ is parallel to the direction $\mathbf{y}$ of the sample. $\mathbf{h}_i$ and $\mathbf{y}$ can be described by cartesian coordinates (h_{i1}, h_{i2}, h_{i3}) and (y_1, y_2, y_3) or by spherical coordinates (ϑ, φ) and (χ, η) with $0 \leq \varphi,\ \eta < 2\pi$, $0 \leq \vartheta,\ \chi \leq \pi$, respectively.

Definition A pole figure is a function $P_{\mathbf{h}_i}(\mathbf{y})$, $\mathbf{y} \in S^2$ that satisfies condition [4],

$$\frac{\mathrm{d}V(\mathbf{h}_i \parallel \mathbf{y})}{V} = P_{\mathbf{h}_i}(\mathrm{y})\mathrm{d}y,$$

here $\mathrm{d}\mathbf{y} = \sin\chi\,\mathrm{d}\chi\,\mathrm{d}\eta$ is a measure on the sphere S^2. The volume of the sample here is also assumed to be equal to the joint volume of all monocrystals. Only the orientation or the crystallites rather than their spatial positions are taken into account. It follows from the definition that $P_{\mathbf{h}_i}(\mathbf{y})$ is a nonnegative and

$$\int_{S^2} P_{\mathbf{h}_i}(\mathbf{y})\mathrm{d}\mathbf{y} = 1.$$

Because of the symmetry of the crystallites for rotations g and $g_{B_j}g$ where $g_{B_j} \in G_B$ is a crystallite symmetry group, the following relation must be fulfilled:

$$P_{\mathbf{h}_i}(\mathbf{y}) = P_{g_{B_j}\mathbf{h}_i}(\mathbf{y}) \tag{40}$$

and if there is sample symmetry,

$$P_{\mathbf{h}_i}(\mathbf{y}) = P_{g_{B_j}\mathbf{h}_i}(g_{A_k}\mathbf{y}), \tag{41}$$

where $g_{A_k} \in G_A$ is the sample symmetry group. If there is some function $P_{\mathbf{h}_i}(\mathbf{y})$, to obey properties (40) and (41) it can be symmetrized as follows:

$$P_{\mathbf{h}_i}(\mathbf{y}) = \frac{1}{N_B}\sum_{j=1}^{N_B} P_{g_{B_j}\mathbf{h}_i}(\mathbf{y}), \quad P_{\mathbf{h}_i}(\mathbf{y}) = \frac{1}{N_A N_B}\sum_{j=1}^{N_B}\sum_{k=1}^{N_A} P_{g_{B_j}\mathbf{h}_i}(g_{A_k}\mathbf{y}).$$

Statement of the problem Given a finite set of unit vectors $\mathbf{h}_i \in S^2$ and a corresponding set of experimentally measured pole figures $P_{\mathbf{h}_1}(\mathbf{y}), \dots, P_{\mathbf{h}_N}(\mathbf{y})$. We want to find the orientation distribution function, $f(g)$. Pole figures are connected with the orientation distribution function as follows:

$$P_{\mathbf{h}_i}(\mathbf{y}) = \hat{P}(\mathbf{h}_i, \mathbf{y}, g)f(g).$$

The next formula presents the explicit appearance of the operator $P(\mathbf{h}_i, \mathbf{y}, g)$ (Matthies (1979)):

$$P_{\mathbf{h}_i}(\mathbf{y}) = \int_0^{2\pi} (f[\mathbf{h}_i, \phi]^{-1}[\mathbf{y}, 0]) + f[-\mathbf{h}_i, \phi]^{-1}[\mathbf{y}, 0])\mathrm{d}\phi. \tag{42}$$

Here $[\mathbf{h}_i, \phi]^{-1}$ denotes the rotation inverse to $[\mathbf{h}_i, \phi]$, which means rotation with Euler angles $\{\vartheta, \varphi, \phi\}$. (First two angles are spherical coordinates of vector $\mathbf{h}_i$.) Formula (42) can be obtained from the fact that the rotation transfering $\mathbf{h}_i$ into $\mathbf{y}$ ($\mathbf{h}_i = g\,\mathbf{y}$) has the appearance $g = [\mathbf{h}_i, \phi]^{-1}\,[\mathbf{y}, 0]$ and ϕ the arbitrary angle from the interval $0 \leq \phi < 2\pi$. Orientation distribution function $f(g)$ can be expanded into the series

$$f(g)=\sum_{l=1}^{\infty}\sum_{m=-l}^{l}\sum_{n=-l}^{l}C_l^{mn}T_l^{mn}(g). \tag{43}$$

An addition theorem is known (see Vilenkin (1968)) for the spherical function,

$$Y_l^{n}(\mathbf{h}_i)=\sum_{m=-l}^{l}Y_l^{m}(\mathbf{y})T_l^{mn}(g).$$

From (42) with expansion (43) using the addition theorem it is possible to obtain a formula that connects the expansion coefficients of the pole figures with the orientation distribution function coefficients:

$$P_{\mathbf{h}_i}(\mathbf{y})=\sum_{l=1}^{\infty}\sum_{m=-l}^{l}\sum_{n=-l}^{l}\frac{4\pi}{2l+1}\frac{1+(-1)^l}{2}C_l^{mn}Y_l^{m}(\mathbf{y})Y_l^{n*}(\mathbf{h}_i). \tag{44}$$

This sum depends only on terms with even indices l. If we write $f(g)$ in the form

$$f(g)=\tilde{f}(g)+\tilde{\tilde{f}}(g),$$

here $\tilde{f}(g)$ corresponds to the part of the expansion (43) with even indices l, $\tilde{\tilde{f}}(g)$ corresponds to the part of the expansion (43) with odd indices l. The operator $\hat{P}(\mathbf{h}_i,\mathbf{y},g)$ acts in such a way that

$$\hat{P}(\mathbf{h}_i,\mathbf{y},g)\tilde{\tilde{f}}(g)=0.$$

In other words, it has nonzero kernel. This is a consequence of the symmetry of the experiment with respect to directions $\mathbf{y}$ and $-\mathbf{y}$ and also $\mathbf{h}_i$ and $-\mathbf{h}_i$. From (44) it follows that there is no information in the pole figures about the odd part of the orientation distribution function $\tilde{\tilde{f}}(g)$. That fundamental fact does not depend on the method used to compute the orientation distribution function but depends only on the information the pole figures are identical. That means that the problem of reproducing the orientation distribution function from measured pole figures is ill-posed (there exist no unique solution). Therefore, only $\tilde{f}(g)$ can be produced from the experimentally measured pole figures.

The most commonly used method to solve the problem is Bunge–Roe method. In 1965, almost at the same time, Roe and Bunge suggested the following method. Expand experimental pole figures into series with spherical harmonics,

$$P_{\mathbf{h}_i}(\mathbf{y}) = \sum_{l=1}^{\infty} \sum_{m=-l}^{l} F_l^m Y_l^m(\mathbf{y}).$$

Coefficients of the expansion (43) are connected with F_l^m. In computations, the least square method is usually used to obtain C_l^{mn}. Using (44) it is possible to obtain the next important formula that connects the pole figures with the coefficients of the orientation distribution function:

$$\sum_{i=1}^{N} W_i \left(F_l^m(\mathbf{h}_i) - \frac{4\pi}{2l+1} \sum_{n=-l}^{l} C_l^{mn} Y_l^n(\mathbf{h}_i) \right) \to \min,$$

where W_i is the weight of the pole figure. The length of the series (43) in practical computations depends on the number of measured pole figures and the symmetry of the crystallite. For example, for cubic symmetry of crystallite with three pole figures $l_{\max} = 22$. In the Bunge–Roe method, coefficients with odd l are assumed to be zero. This is the reason why a computed orientation distribution function has negative values and false maxima (ghost phenomena). This was noticed by many scientists but was interpreted as computational errors (errors because of calculation of coefficients $C_l^{m,n}$, errors of summation and truncation of the series). Matthies (1979) showed that the ghost phenomena and negative values are in fact due to the incompleteness of the information contained in the pole figures. At present several improved methods to find an orientation distribution function are known.

Our idea for the solution of that problem is the following. It happens that the circular normal distribution on the SO(3) group and the sphere S^2 are connected to each other by the integral relation (42). We suggest approximating the experimentally measured pole figures by a linear combination of normal distributions on S^2 by means of fitting variance like parameters and weights. This will be a nonlinear problem about unknown parameters. The orientation distribution function is taken as a linear combination of normal distributions with parameters and weights found. As the odd part of the orientation distribution function we assume odd part of the sum obtained in this way. Examples of such an approach can be found in Bukharova *et al.* (1988), Bukharova and Savyolova (1993), Nikolayev *et al.* (1992). It must be mentioned that also several other methods how to approximate the odd part have been suggested. For a survey see, e.g., Wagner and Dahms (1991).

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