About normal distribution on SO(3) group in texture analysis

T I Savyolova¹, S V Filatov¹

¹ National Research Nuclear University MEPhI, Kashirskoe highway, 31, 115409, Moscow, Russia
E-mail: feelshadow5@gmail.com

Abstract. This article studies and compares different normal distributions (NDs) on SO(3) group, which are used in texture analysis. Those NDs are: Fisher normal distribution (FND), Bunge normal distribution (BND), central normal distribution (CND) and wrapped normal distribution (WND). All of the previously mentioned NDs are central functions on SO(3) group. CND is a subcase for normal CLT-motivated distributions on SO(3) (CLT here is Parthasarathy’s central limit theorem). WND is motivated by CLT in $\mathbb{R}^2$ and mapped to SO(3) group. A Monte Carlo method for modeling normally distributed values was studied for both CND and WND. All of the NDs mentioned above are used for modeling different components of crystallites orientation distribution function in texture analysis.

1. Introduction
There are a number of different approaches for calculating crystallites orientation distribution function (CODF) of polycrystalline materials by obtaining the sample of pole figures (PF) using X-ray or neutron methods or by using EBSD (Electron Backscattering Diffraction) methods [1-4]. One of those methods is a components method or standard function approximation method [3, 4]. Different distributions are used as central functions, but the most attractive ones are normal distributions on SO(3) group [4-7]. Articles [8, 11, 12] introduce a new kind of ND on SO(3) group. Article [8] compares (numerically and by properties) known NDs on SO(3), which are central functions and are able to be presented as characters of representations of SO(3) group. Articles [9-10] also review and compare known NDs on SO(3) group.

This article conducts the comparison between that kind of NDs on SO(3). Normal distributions are computed for different values of concentration parameter, asymptotic behaviour is analysed for small values of concentration parameter, the presence of properties characteristic for normal distributions on SO(3) group is studied. As well as the possibility of applying these NDs in texture analysis is considered. That includes computational complexity of the algorithm and the correctness of application of Monte Carlo method for modeling the EBSD experiment for studied NDs.

2. Central normal distributions on SO(3) group
Central functions on SO(3) can be expressed as a series with terms as characters of representations of SO(3) group

$$\chi_l(t) = \frac{\sin[t(l + \frac{1}{2})]}{\sin(\frac{t}{2})}, \quad l = 0, 1, \ldots, \quad t \in (-\pi, \pi]$$

that form and orthogonal function system with respect to the invariant measure [11].
dq = \frac{1}{\pi} \sin^2 \left( \frac{t}{2} \right) dt

3. Normal distributions
The article studies following distributions:

3.1. Fisher normal distribution (FND)
\frac{e^{k_F^2 \text{cos}(t)}}{I_0(k_F^2) - I_1(k_F^2)} \frac{1}{\pi} \sin^2 \left( \frac{t}{2} \right) \tag{1}

I_0(z), I_1(z) - modified Bessel functions.

3.2. Bunge normal distribution (BND)
C(k_B) \exp \left( - \frac{k_B^2 t^2}{2} \right) \frac{1}{\pi} \sin^2 \left( \frac{t}{2} \right) \tag{2}

C(k_B) – normalization constant.

3.3. Central normal distribution (CND)
\sum_{l=0}^{\infty} (2l + 1) \exp \left( \frac{-l(l - 1)}{2k_C^2} \right) \frac{\sin((l + \frac{1}{2})t)}{\sin(t/2)} \frac{1}{\pi} \sin^2 \left( \frac{t}{2} \right) \tag{3}

3.4. Wrapped normal distribution (WND)
\sum_{l=-\infty}^{+\infty} \frac{k^3}{\sqrt{2\pi}} (2lt - t)^2 \exp \left( -\frac{k^2 (2lt - t)^2}{2} \right) \tag{4}

Figure 1. Fisher normal distribution
Figure 2. Bunge normal distribution
Figure 3. Central normal distribution

Figure 4. Bunge normal distribution

Distributions (1)-(3) were used as model functions in texture analysis before [1-7]. WND (4) is a recently introduced ND, obtained as a result of modeling a Markov chain using Monte Carlo method on SO(3) group [8].

In ([8], p. 4) distribution (4) is explained as distributional limit for compositions of large numbers of independent, small random rotations and it is pointed out that WND statistically corresponds to Maxwell-Boltzmann distribution.

WND is motivated by CLT in $R^3$ and converted to SO(3) group through exponential mapping.

Let’s point out main properties of distributions (1)-(4):

- FND and BND are able to give the best likelihood estimation (maximum likelihood estimation method, that is used in statistics to define unknown parameters of a model by the sample) and able to maximize entropy [2].
- CND is an infinitely divisible distribution [6]. It has a CLT motivation (CLT here is Parthasarathy’s central limit theorem on SO(3) group) and is able to be obtained as a result of Brownian motion.
- WND is obtained as a result of modeling a Markov chain using Monte Carlo method on SO(3) group.

Figures 1-4 show plots of distributions (1)-(4) for $k = 2^m, m = 0,1,2,3$.

4. Asymptotic analysis of different NDs on SO(3) group

Let’s take WND (4). With $l = 0$ expression (4) transforms into

$$f(t)dt = \frac{k^3}{\sqrt{2\pi}} t^2 e^{-\frac{k^2 t^2}{2}} dt, \quad |t| < \pi$$

(5)

With the $k^2 t^2 = u$ variable substitution in (5) it turns into

$$f_1(t)dt = \frac{1}{2\sqrt{2\pi}} \frac{1}{u^{\frac{3}{2}}} e^{-\frac{u}{2}} du$$

(6)

Distribution (6) coincides with $\chi^2_3$ distribution (with 3 degrees of freedom). Using the table of $\chi^2$ values ([14], p.572), it was found out that with the value of concentration parameter $k$ and confidence interval corresponding to expressions (7)
only one term (5) of the series (4) approximates WND with the p-value (confidence value) of $\beta = 0.95$.

With that said, it should be mentioned, that previously introduced WND plot (figure 4) displays wrapped normal distribution calculated using expression (5) for $k^2 = 2, 4, 16$. And uses expression (4) for $k^2 = 1$ considering only the terms that correspond to $l = -1, 0, 1$.

To create a CND plot (figure 3) only first 100 terms of the series (3) were used to calculate the distribution.

Article [6] states that expression \(8\) approximates CND (where $\varepsilon^2 = \frac{1}{2k^2}$)

\[
f(t)dt = \frac{\sqrt{\pi}}{e^{\varepsilon^2}} \text{erfc} \left( \frac{\varepsilon}{2} \right) \exp \left( \frac{t^2}{4\varepsilon^2} \right) \frac{1}{2} \sin \left( \frac{t}{\sqrt{2}} \right) dt, \quad |t| \leq \pi
\]  

With $\frac{t^2}{2\varepsilon^2} = u$ substitution, and as $t \to 0$, (8) transforms into

\[
f(u)du = \frac{1}{2} e^{\frac{1}{2\varepsilon^2}} \text{erfc} \left( \frac{1}{2\sqrt{2k}} \right) f_{\chi^2_3}(u)du
\]

Using the same variable substitution $k^2 \varepsilon^2 = u$ and taking into account $t \to 0$, it can be shown that FND and BND are approximated by $\chi^2_3$ distribution with three degrees of freedom.

- **FND**

\[
f(u)du = e^{k^2 \frac{1}{2\varepsilon^2}} \frac{\sqrt{2\pi}}{8\pi k^3 (I_0(k^2) - I_1(k^2))} f_{\chi^2_3}(u)du
\]

- **BND**

\[
f(u)du = C(k) \frac{\sqrt{2\pi}}{8\pi k^3} f_{\chi^2_3}(u)du
\]

Figures 5a and 5b show plots for separate terms ($l = 0, \pm 1, ...$) of the series (4) with $k = 2$, $k = \frac{3}{4}$ and $-\infty < t < +\infty$.

**Figure 5.** WND separate terms a) k=2 b) k=0.75

Figure 5a shows, that for $k = 2$ each plot of each term appears to be almost isolated from the others with the period of $2\pi$. In that case the conditions (7) are met and it is enough to use only one
term of series (4), where \( l = 0 \), to calculate WND for \( |t| \leq \pi \). On the other hand, figure 5b shows that for \( k = \frac{3}{4} \) plots seem to intersect with each other, therefore the influence of the “neighbor” terms has to be accounted for.

In that case, it is sufficient to use two terms of series (4) (where \( l = 0, 1 \)) to calculate WND. That is because on \( [0; \pi] \) the term corresponding to \( l = 0 \) gives a 0.5 of the “weight” of the whole function, whereas the term corresponding to \( l = 1 \) gives the remaining part of “weight” (see the table of \( \chi^2 \) values with 3 degrees of freedom: for \( k = \frac{3}{4} \) the confidence interval \( |t| \leq \left( \frac{3}{2} \right)^2 \approx 2.46 \), and the possibility \( p = \frac{1}{2} \) ([14], p.572). It becomes obvious, that for \( k \geq 2 \) it is possible to use only one term corresponding to \( l = 0 \) in order to calculate WND, however, for \( k \leq \frac{1}{2} \) two or more terms have to be used for the same purpose.

5. Monte Carlo method

Monte Carlo methods for calculating ND on SO(3) group could be used to model orientations of separate crystallites of polycrystalline materials [4]. These distributions are convenient to use in EBSD (Electron Backscattering Diffraction) experiment in order to study the texture of a material’s microstructure as well as its macrostructure [4, 8].

Article [4] introduces Monte Carlo method for calculating ND’s on SO(3) based on Parthasarathy’s CLT. Article [8] describes Monte Carlo method for calculating WND based on CLT in \( R^2 \) and mapping to SO(3) group.

Let’s study the examples of Monte Carlo method application for calculating CND [4] and compare modeling results with WND. The calculations were carried out for \( \varepsilon = 1.4 \) (\( \varepsilon^2 = \frac{1}{2k^2} \)), with sample size \( N = 10^4 \), number of convolutions \( n = 20 \) and number of bins in a histogram \( n_{Bins} = 30 \).

The following results were obtained after applying the Monte Carlo method and calculating Pearson’s test statistic:

![Figure 6. CND \( \varepsilon = 1 \).](image1)

![Figure 7. CND \( \varepsilon = \frac{1}{4} \).](image2)
In the case depicted by figure 6 Pearson’s test statistic W = 25.55 does not exceed the critical value of $\chi^2 = 42.56$. Therefore the hypothesis (that there is no difference between theoretical distribution and experimental distribution of the sample) is accepted.

In the case depicted by figure 7 Pearson’s test statistic W = 21.77 does not exceed the critical value of $\chi^2 = 42.56$. Therefore the hypothesis (that there is no difference between theoretical distribution and experimental distribution of the sample) is accepted.

In the case depicted by figure 8 Pearson’s test statistic W = 180.21 exceeds the critical value of $\chi^2 = 42.56$. Therefore the hypothesis (that there is no difference between theoretical distribution and experimental distribution of the sample) is rejected.

In the case depicted by figure 9 Pearson’s test statistic W = 26.78 does not exceed the critical value of $\chi^2 = 42.56$. Therefore the hypothesis (that there is no difference between theoretical distribution and experimental distribution of the sample) is accepted.

To sum up, for CND the hypothesis is accepted for all of the considered values of $\varepsilon$ ($\varepsilon = 1, \frac{1}{2}$), however for WND, the hypothesis is accepted only in the case of $\varepsilon = \frac{1}{4}$, while for $\varepsilon = 1$ it is rejected according to Pearson’s chi-squared test.

Hence it can be concluded that CND and WND approximate each other for small values of $\varepsilon$ and differ otherwise (or approximate each other for large values of concentration parameter $k$ and differ otherwise).

6. Texture analysis application

Normal distributions on SO(3) are widely used in texture analysis to solve problems of CODF restoration by its PF [1-7]. CODF is presented as a sum of ND’s with certain weights. Articles [1] use ND (2), [3, 6] – ND (1). Article [8] suggests using WND (4) for same purposes.

PF for CND (3) is calculated as follows ([4], p.106):

$$P_n(\vec{y}, q_0, \varepsilon) = \sum_{l=0}^{\infty} (2l + 1) \exp(-l(l + 1)\varepsilon^2) P_l(\vec{h}, q_0\vec{y})$$

(9)

where $\vec{h}$ - desired crystallographic direction, $q_0 \in SO(3)$ - center of ND, $\vec{y} \in S^2$ – point on two-dimensional sphere, $\varepsilon$ – concentration parameter ($k \leq \frac{1}{\varepsilon}$), $P_l(z), l = 0,1, ...$ - Legendre polynomials.

With $\varepsilon \to 0$ + PF (9) is approximated by expression (8)

$$P(\cos\theta)\sin\theta d\theta \approx \frac{1}{\varepsilon^2} \exp\left(\frac{\theta^2}{4\varepsilon^2}\right)\theta d\theta$$

(10)

In the light of the fact that with $t \to 0$ + ND (3) and ND (4) approximate each other, expression (10) can be used to closely calculate PF for large values of $k$ (small values of $\varepsilon$).
Presenting WND (4) as a series of terms, where terms themselves are characters of representations of SO(3) group, and using ([15], p. 509), values of coefficients are calculated as

\[ C_l = \left( 1 + \frac{l^2}{k^2} \right) \exp \left( -\frac{l^2}{2k^2} \right) - \left( 1 + \frac{(l + 1)^2}{k^2} \right) \exp \left( -\frac{(l + 1)^2}{2k^2} \right) \]

Thus WND (4) has a significant difference from CND (3) in presenting it as a series with terms as characters of representations of SO(3) group.

Article [16] gives an example of CODF approximation for texture description using just one component of CND (3). The texture was obtained as a result of deformation of monocrystalline alloy Ni-Ti. Two pole figures were used to obtain the parameters of CND: center coordinates \( \theta_0 = (56.92^\circ, 75.89^\circ, 65.78^\circ) \) (Euler rotation angles), component weight \( M_0 = 1.51 \), concentration parameter \( \varepsilon = 0.025 \) \( \varepsilon^2 = (2k^2)^{-1} \). Figure 10 depicts the kind of PF that corresponds to expression (10) without measure \( \sin \theta d\theta \) and only its even part, because it is well known that CODF reconstructs ambiguously ([4], p. 96).

![Figure 10. Pole figure](image)

Figure 10 has R in degrees plotted on the x-axis. Stars on figure 10 correspond with experimentally measured PF \{110\} values obtained by X-ray method, solid line represents calculated results.

Each of the NDs (1)-4 can be equally used as a model function for CODF approximation due to their close similarity for the large values of concentration parameter \( k \).

Article [8] presents confidence intervals for concentration parameter \( k \) for different values of \( p \)-value (or confidence value), in order to consider them when EBSD measurements are analyzed. EBSD measurements produce a set of crystallite orientations in polycrystal. That set allows to identify different structure and texture characteristics of a material. Very rarely a material has a texture that could be characterized by CODF similar to the one mentioned before in Ni-Ti example. Mostly texture is characterized by a number of components, including the axial ones [1, 3, 4, and 6]. Which is why it seems doubtful that confidence intervals presented in [8] would find its practical use.

7. Conclusion
This article considers normal distributions on SO(3) group that are able to be represented as central functions [13]. Distributions (1)-(3) are broadly used in texture analysis for modeling crystallite orientation distribution function ([1-7]). Articles [8, 11 and 12] introduce wrapped normal distribution
(4). WND (4) is compared with distributions (1)-(3), and properties, connected with the notion “normal” (the one in probability theory and mathematical statistics on SO(3) group) are analyzed.

WND (4) is characterized by four parameters. Three of them define the position of the “center” and the fourth is the concentration parameter. WND (4) is motivated by CLT that was obtained by consecutive rotations of two-dimensional sphere \( S^2 \) on a small angle uniformly distributed on \( (-\pi; \pi] \).

This article studies how many terms of series (4), depending on the value of parameter \( k \), are needed to obtain a credible result when calculating WND. It appears that for \( \sqrt{\frac{k}{\pi}} \) it is sufficient to use only one term of the series (4) (when \( l = 0 \) to calculate an accurate result with p-value (or confidence value) 0.95.

Monte Carlo method was studied for both CND and WND. The results show that according to Pearson’s chi-squared test for WND (4) the hypothesis is accepted for small values of \( \varepsilon \), for large values it is rejected. (Hypothesis read as follows: there is no difference between theoretical distribution and experimental distribution of the sample.) For CND hypothesis is accepted for all the values of \( \varepsilon \). Which prompts a conclusion, that CND and WND approximate each other for small values of \( \varepsilon \). Not so otherwise.

CND (3), unlike WND (4), is only a subcase of a normal distribution on SO(3) group that is characterized by 9 parameters: the position of the “center” and positive semi-definite \( 3 \times 3 \) matrix (analogue of a covariance matrix) [5].

Let’s point out that corresponding definitions of ND and CLT are provided for a bigger class of groups – SO(n) groups (\( n \geq 2 \)). And for that class of groups Monte Carlo method has been developed in order to solve different problems in texture analysis connected with studying the results of EBSD experiment [4, 6].

The article also shows that FND (1) and BND (2) could also be approximated by \( \chi^2 \) for small values of parameter \( t \).

In conclusion, it is important to mention that all of the studied distributions (1)-(4) can be used to solve different problems in texture analysis.

8. References
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