Estimation of accuracy of kernel and projective methods of probability density distribution restoration from individual orientations on group SO(3)

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In recent years the automation of EBSD systems allows to get a large data of individual crystallographic orientation measurements for investigation of the global texture. The statistical accuracy of the orientation distribution function (ODF) calculation on the basis of EBSD data is actual problem for investigation [1].

The kernel and projective methods for ODF restoration from sample of individual orientations on group $SO(3)$ are investigated. The analytical and numerical calculations of dependence of accuracy for kernel and projective methods from different parameters are considered [2,3].

1. Generalization of Rosenblatt – Parzen method for reconstruction of probability density function on group SO(3)

Denote $g = \{\varphi, \theta, \psi\} \in SO(3)$, $-\pi < \phi, \ \psi \le \pi$, $0 \le \theta \le \pi$, $g^i = \{\phi^i, \ \theta^i, \ \psi^i\}$, $i = 1,...,N$ - is a sample of independent rotations corresponding to probability density function $f(g)$ on group $SO(3)$.

Estimator of function $f(g)$

$$f_N^*(g) = \frac{1}{N(h_N)^3} \sum_{i=1}^{N} q_1\left(\frac{\phi - \phi^{(i)}}{h_N}\right) q_2\left(\frac{\cos\theta - \cos\theta^{(i)}}{h_N}\right) q_3\left(\frac{\psi - \psi^{(i)}}{h_N}\right), \tag{1}$$

where q_i, $i = 1,2,3$ are smoothing kernels. We have

$$f_N^*(g) = f_N(g) + \zeta_N(g), \ f_N(g) = Mf_N^*(g), \ \ \zeta_N(g) \sim N\left(0, d\sqrt{f(g)} \Big/ \sqrt{N(h_N)^3}\right), \tag{2}$$

$$d^2 = \int\limits_{SO(3)} \prod_{i=1}^{3} q_i^2 dg,$$

where operator $Mf(g)$ is the mean value of $f(g)$ and $N(a,\sigma)$ is the normally distributed function.

We have $f_N(g) \to f(g)$ when $N(h_N{}^3) \to \infty, \ N \to \infty, \ h_N \to 0,$ if $\partial^2 f / \partial x_i \partial x_j$ are bounded, where $x_1 = \varphi, \ x_2 = \cos\theta, \ x_3 = \psi.$

Let

$$\Delta_N{}^2 = M \int\limits_{SO(3)} \left| f(g) - f_N^*(g) \right|^2 dg. \tag{3}$$

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We have $$\min_{h_N} \Delta_N = O\left(N^{-2/7}\right) \text{ when } h_N = O(N^{-1/7}). \quad (4)$$

2. Projective methods on group SO(3)

Estimator for coefficients is given by well known formula

$$\hat{C}^l_{mn} = (2l+1)\frac{1}{N}\sum_{i=1}^{N}\overline{t^l_{mn}(g_i)},\ \hat{f}_N(g) = \sum_{l=0}^{L}\sum_{m,n=-l}^{l}\hat{C}^l_{mn}t^l_{mn}(g). \quad (5)$$

Estimator (5) is non bias, consistent, but not robust corresponding to contamination of elements of sample.

Let be $$\Delta^2 = M\int_{SO(3)}\left[\hat{f}_N(g) - f(g)\right]^2 dg = M\Delta_1^{\ 2} + \Delta_2^{\ 2}, \quad (6)$$

$M\Delta_1^{\ 2} = \sum_{l=0}^{L}\sum_{m,n=-l}^{l} D\hat{C}^l_{mn}$ - is variance of Δ_1^2 for independent g^i, $i = 1,...,N$,

$\Delta_2^{\ 2} = \sum_{l=L+1}^{\infty}\sum_{m,n=-l}^{l}\left|C^l_{mn}\right|^2$ is systematic error.

For central functions $$f(t) = \sum_{l=0}^{\infty} C^l\chi_l(t),\ \chi_l(t) = \frac{\sin(l+1/2)t}{\sin(t/2)},\ -\pi \le t < \pi, \quad (7)$$

$$\hat{C}^l = \frac{1}{N}\sum_{i=1}^{N}\chi_l(t_i),\ \ \hat{f}_N(t) = \sum_{l=0}^{L}\hat{C}^l\chi_l(t),\ M\Delta^2 = M\Delta_1^{\ 2} + \Delta_2^{\ 2},\ M\Delta_1^{\ 2} = \sum_{l=0}^{L}\frac{1}{N}\left\{\left(\sum_{l'=0}^{2l} C^{l'}\right) - \left(C^l\right)^2\right\},$$

$$\Delta_2^{\ 2} = \sum_{l=L+1}^{\infty}\left|C^l\right|^2.$$

3. Numerical examples

We use the statistical simulation of normal distribution defined by the central limit theorem to get the sample with individual orientations.

The central normal distribution (CND) is written by formula

$$F(t)dt = \sum_{l=o}^{\infty}(2l+1)\exp\left\{-l(l+1)\varepsilon^2\right\}\frac{\sin(l+1/2)t}{\sin(1/t)}\frac{1}{\pi}\sin^2\frac{t}{2}dt,\ -\pi \le t < \pi. \quad (8)$$

3.1. Kernel smoothing of individual orientations

For smoothing of individual orientations we used the Gauss kernel. In figure 1 the smoothed (continuous line) results and the results by summing of Fourier series (dotted line) $F(t)$ are represented with parameters $\varepsilon^2 = 1$ (figures 1a), $\varepsilon^2 = 1/4$ (figures 1b), $\varepsilon^2 = 1/64$ (figures 1c) with sample size $N = 3\times10^3$. When one increases the sample size from *N*=500 to $N = 3\times10^3$ the relative error decreases from 5% to 2,5% in maximum of CND with $\varepsilon^2 = 1/4$ and it decreases from 27% to 24% for CND with $\varepsilon^2 = 1/64$.

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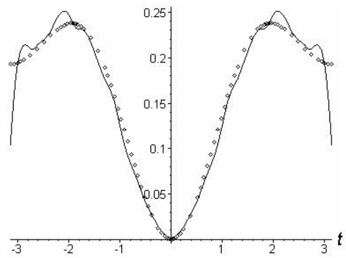

Fig. 1a

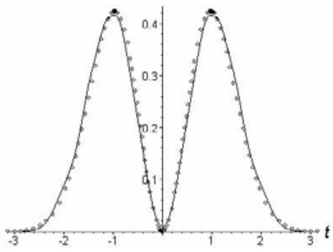

Fig. 1b

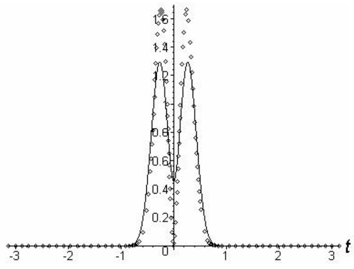

Fig. 1c

Table 1

Δ_N	ε^2		
	1/4	1/16	1/64
0,10	237	1142	5718
0,01	4199	20294	102670

In table 1 it is considered the value of sample size *N* for optimal h_N by minimizing Δ_N (4) for CND with different parameter ε^2.

3.2. Comparison of different smoothing kernels

We compare the different kernels for smoothing of individual orientations for CND [4]

a) Gauss kernel $q_1(t) = C_1 \exp\left(-t^2/4\right)$;

b) $q_2(t) = C_2 \left\{\cos(t/2)\right\}^{2k}, k = 2$;

c) Epanechnikova kernel $q_3(t) = C_3\left(1-(t/h)^2\right),\ |t| \le h.$

$C_i,\ i = 1,2,3$ are normalized constants $C_i \int_{-\pi}^{\pi} q_i(t)\,dt = 1$.

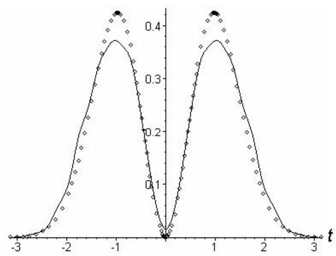

Fig. 2a

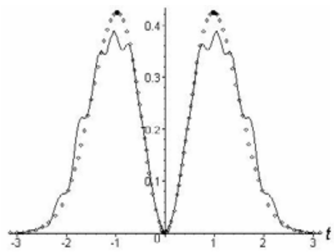

Fig. 2b

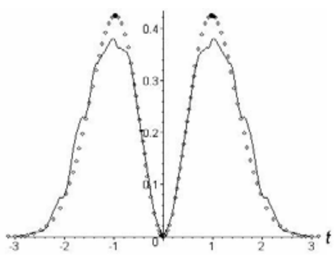

Fig. 2c

In figures 2a – 2c are shown the results of smoothing by kernels a) – c) the orientations for CND with $\varepsilon^2 = 1/4$ with sample size *N*=500. We can see that the results with kernels $q_2(t)$ and $q_3(t)$ are better than with Gauss kernel.

3.3. The influence of errors for smoothing of orientations

We consider the individual orientations for CND with parameter $\varepsilon^2 = 1/16$ with simulated errors $\tilde{t}_i = t_i + \delta\xi_i,\ i = 1, \ldots, N$, where ξ_i is uniformly distributed in interval $(-1;1)$ and ξ_i is normal distributed $N(0,1)$. δ is equal to 0,01; 0,1; 0,3.

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The relative error is equal to 6%, 20% and 34% when the orientation error δ=0,01; 0,1 and 0,3 correspondently. It is calculated in maximum of CND with parameter $\varepsilon^2 = 1/16$ with sample size N=500.

3.4. Projective methods

We use the statistical simulation of normal distribution to get the sample with individual orientations (we simulated distribution with parameters $\varepsilon^2 = 1,\ 1/16,\ 1/64$). Then we calculate coefficients $\hat{C}^l$ and function $\hat{F}_N(t)$ using formulas (7), (8).

Table 2.

N \ l	$\varepsilon^2 = 1/4$			$\varepsilon^2 = 1/64$		
	1	3	4	1	10	17
100	3%	50%	6600%	1%	30%	82%
1000	3%	37%	606%	0,20%	12%	14%

For CND the dependence of relative error $\Delta_C = \left(\left|C^l - \hat{C}^l\right|\right)/C^l$ for coefficient estimation from sample size N and from number l is written in table 2.

Summary

The next results follow from given investigations:

- the asimptotic degree of convergence is equal to $O(N^{-2/7})$ in sense of mean square convergence for kernel methods on SO(3), when the optimal parameter of smoothing $h_N = O(N^{-1/7})$.
- the approximation accuracy of kernel methods depends from the choice of smoothing kernel. From numerical examples we have that the best results give the kernels $q_2(t)$ and $q_3(t)$.
- the accuracy of $f(g)$ calculation by projective methods depends from sample size, number of Fourier coefficient, analog of dispersion (parameter ε^2 for CND). It is determined by choice of number of Fourier series members L for summing.
- the numerical experiments give the statistical regularity of kernel and projective methods for reconstruction of $f(g)$ corresponding to individual orientation error, when error is small enough (for example, δ =0,01 – 0,05 for CND with ε=1/4).

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