STATISTICS FOR INDIVIDUAL ORIENTATION MEASUREMENTS

Statistics for orientations

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Abstract

A new class of distributions for data from crystal orientation measurements is introduced. This class characterizes its distributions by their low order harmonics up to arbitrary order, and adds harmonic functions of higher order according to the assumption of maximum entropy. This yields a strictly positive distribution density function, which can easily be handled by powerful statistical procedures well known from other sciences. This framework provides solutions to various tasks: Does the ODF follow a given distribution model? Are two sample textures similar? What are the statistical errors of experimental harmonic coefficients? How to simulate from a sample ODF? It also provides models for regression of textures: The variation of texture according to the variation of a controlling parameter.

Keywords: measurement error, OIM, statistics, texture regression models

1 A distributional model for orientations

The ODF is a density of a distribution on the group SO_3 of orientations. We introduce a family of distributions $ExpRot[L, \overset{:}{G}, \dot{G}; (\theta_\tau)_{\tau \in \overset{:\cdot}{I}(L)}]$ defined by a degree L of a series expansion, the crystal symmetry group $\overset{:}{G}$, the sample symmetry group $\dot{G}$, and a set of real valued parameters $\theta_\tau,\ \tau \in \overset{:\cdot}{I}(L)$, by its distribution density:

$$f_\theta(g) = A(\theta)\exp\left(-\sum_{l=1}^{L}\sum_{\mu=1}^{M(l)}\sum_{\nu=0}^{N(l)} \theta_l^{\mu\nu}\, \overset{:\cdot}{T}{}_l^{\mu\nu}(g)\right) = A(\theta)\exp\left(-\sum_{\tau \in \overset{:\cdot}{I}(L)} \theta_\tau\, \overset{:\cdot}{T}_\tau(g)\right)$$

(Beran 1979) introduced a similar family for the distributions of directions. This family has some interesting properties:

- These are the distributions of maximum entropy given a series expansion up to order L.[1] The coefficients

$$C_l^{\mu\nu} = E[\ddddot{T}_l^{\mu\nu}(g)] = \oint f_\theta(g)\,\ddddot{T}_l^{\mu\nu}(g)dg,\; l = 1, \ldots, L$$

  characterize a distribution in $ExpRot[L, \overset{\vdots}{G}, \dot{G}; (\theta_\tau)_{\tau \in \ddddot{I}(L)}]$ uniquely.
- All distributions in $ExpRot[\ldots]$have strictly positive distribution densities.
- The maximum likelihood estimation factorizes over the empirical harmonic components $\hat{C}_l^{\mu\nu}$ given later in the text.
- Given the harmonic components of the density up to a given degree L, harmonic components of higher order will be added such that we get a positive distribution density which maximizes the entropy of the distribution.
- If the energy $Q(g)$ of a grain with orientation g is given by a function in terms of low order harmonics:

$$Q(g) = \sum_{l=1}^{L} \sum_{\mu=1}^{M(l)} \sum_{\nu=0}^{N(l)} \tilde{\theta}_l^{\mu\nu}\,\ddddot{T}_l^{\mu\nu}(g)$$

  and the probability of a specific rotation g is governed by Gibbs dynamics, then the correct distribution would be: $ExpRot[L, \overset{\vdots}{G}, \dot{G}; \tilde{\theta}]$.
- In the case of no sample symmetry ($\dot{G} = \{1\}$) the model is rotationally invariant for all L.
- The model $ExpRot[L, \overset{\vdots}{G}, \dot{G}; \cdot]$ is a strict sub-model of the related models $ExpRot[L', \overset{\vdots}{G}, \dot{G}; \cdot]$ and $ExpRot[L, \overset{\vdots}{G}, \dot{G}'; \cdot]$, where $L < L'$ and $\dot{G} \subset \dot{G}'$.
- The models $ExpRot[L, \overset{\vdots}{G}, \dot{G}; \cdot],\ L \in \mathbb{N}$, are dense in the space of all continuous distribution on SO_3 with the symmetry properties described by $\overset{\vdots}{G}$ and $\dot{G}$, i.e. we can approximate any distribution arbitrarily well, if we only choose L large enough.
- For all $\theta_l^{\mu\nu} \in \mathbb{R}$ there exists an $A(\theta)$ such that $ExpRot[\ldots; \theta]$ yields a valid probability density.
- There is a one to one relation between the parameters θ and the harmonic components $C_l^{\mu\nu}$ of the density. $C_l^{\mu\nu}$ is the expected value of $\ddddot{T}_l^{\mu\nu}(g)$ under the parameter θ, and $\hat{\theta} = \theta$ is the ML-estimation of the parameter θ under observed $\hat{C}_l^{\mu\nu} = C_l^{\mu\nu}$.
- Since this distribution density has no negative parts, it represents a true distribution. Orientations with this distribution can be simulated.
- The Fisher-matrix-distribution is equal to $ExpRot[1, \{1\}, \{1\}, \theta]$.

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[1] Assuming a nonstandard normalisation: $\oint \ddddot{T}_l^{\mu\nu}(g)^2 = 1$

2 Maximum Likelihood Estimation

Because these families are special cases of regular exponential families some powerful statistical tools are available (assuming you have a fast computer). The maximum likelihood estimator $\hat{\theta}$ of θ is given by the equation:

$$E_{\hat{\theta}}(\ddot{T}_l^{\mu\nu}(g)) = \hat{C}_l^{\mu\nu}, \text{ where} \tag{1}$$

$$\hat{C}_l^{\mu\nu} := \frac{1}{n}\sum_{i=1}^{n} \ddot{T}_l^{\mu\nu}(g_i), \quad g_i = \text{orientation of grain } i$$

is the sample mean of the harmonic functions. The derivative of the $E_\theta[\ddot{T}_l^{\mu\nu}(g)]$ is given by:

$$\frac{d(E_\theta(\ddot{T}_l^{\mu\nu}(g)))_{l\mu\nu}}{d\theta} = Var_\theta\left((\ddot{T}_l^{\mu\nu}(g))_{l\mu\nu}\right)$$

$E_\theta(\ldots)$ and $Var_\theta(\ldots)$ can be calculated for every θ by numerical integration:

$$Q(g) := \sum_{l=1}^{L}\sum_{\mu=1}^{M(l)}\sum_{\nu=0}^{N(l)} \theta_l^{\mu\nu}\, \ddot{T}_l^{\mu\nu}(g) \tag{2}$$

$$A(\theta) := \left(\oint_{SO_3} \exp\left(-Q(g)\right) dg\right)^{-1} \tag{3}$$

$$E_\theta(\ddot{T}) = A(\theta) \oint_{SO_3} \ddot{T}(g) \exp\left(-Q(g)\right) dg \tag{4}$$

$$Var_\theta(\ddot{T}) = A(\theta) \oint_{SO_3} \ddot{T}(g)\, \ddot{T}(g)^t \exp\left(-Q(g)\right) dg - E_\theta(\ddot{T})E_\theta(\ddot{T})^t \tag{5}$$

where $\ddot{T}(g) = (\ddot{T}_l^{\mu\nu}(g))_{l\mu\nu}$ is used as a vector valued function. The maximum likelihood estimator $\hat{\theta}$ can then be calculated by solving the equation (1) using the Newton algorithm. The maximized likelihood is given by:

$$\mathrm{L}(\hat{C}_l^{\mu\nu}; \hat{\theta}) = A(\hat{\theta})^n \exp\left(-n \sum_{l=1}^{L}\sum_{\mu=1}^{M(l)}\sum_{\nu=0}^{N(l)} \hat{\theta}_l^{\mu\nu} \hat{C}_l^{\mu\nu}\right) \tag{6}$$

The solution is unique, as the continuously differentiable function $E_\theta[\ddot{T}]$ is strictly convex. Therefore, Newton's algorithm will converge to the proper solution. The estimated asymptotic estimation variances of the estimated coefficients θ and C are given by:

$$\widehat{Var}(\hat{\theta}) = \frac{1}{n} Var_{\hat{\theta}}(\dddot{T})^{-1}, \quad \widehat{Var}(\hat{C}) = \frac{1}{n} Var_{\hat{\theta}}(\dddot{T}) \qquad \textbf{(7)}$$

where n is the number of measured crystal grains. Thus our model provides standard estimation errors for the harmonic coefficients. The maximum likelihood estimator exists if and only if $\hat{C}$ is in the interior of the convex hull of the possible values for $\dddot{T}$.(Johansen 1979) This holds with probability one if more grains are measured than parameters are in the model.

3 Models and Tests

The model is a full distributional model. Therefore we can test, if the data, which we have, is compatible with a given distribution model. Further we can ask how strong the departure from the model is and how exact we can estimate this departure and we can give confidence regions for models. Only some basic test will be outlined here.

The general theory of exponential families provides a construction scheme of a powerful test for the comparison of a model M_0 with a supermodel $M_1 \supset M_0$ (Witting 1995). This test is called likelihood ratio test. For the test problem

$$H_0 : \mathit{ODF} \in M_0 \quad vs. \quad H_1 : \mathit{ODF} \in M_1$$

the test statistic

$$D := 2 \ln \frac{L_1(\hat{C}; \hat{\theta}^{(1)})}{L_0(\hat{C}; \hat{\theta}^{(0)})} \qquad \textbf{(8)}$$

is asymptotically distributed χ^2_d, where d represents the number of parameters added from model M_0 to model M_1. $\hat{\theta}^{(i)}$ denotes the maximum likelihood estimator for model $M_i,\ i = 0, 1$. L_i denotes the likelihood function for model $M_i,\ i = 0, 1$. The test does not reject the hypothesis H_0, if the test statistic D is lower than the 0.95-quantile of the χ^2_d-distribution. This test is valid only for a big size of n ($> 30 * |\dddot{I}(L')|$), because the χ^2-approximation is valid only for large n.

3.1 Testing for the necessary degree L

In the most simple case we assume to know that the data stems from a distribution of this type but with high degree L'. Thus we want to test whether the data is sufficiently well represented by harmonic coefficients up to order L and the additional information that the data is compatible with the model $\mathit{ExpRot}[L, \vdots{G}, \dot{G}; \cdot]$, against the alternative that we have to use more harmonic coefficients. Thus we get the test problem:

$$H_0 : \mathit{ODF} \in \mathit{ExpRot}[L, \vdots{G}, \dot{G}; \cdot] \ vs.\ H_1 : \mathit{ODF} \in \mathit{ExpRot}[L', \vdots{G}, \dot{G}; \cdot], L' > L$$

Since the alternative is an exponential superfamily of the hypothesis, we can use the likelihood ratio test.

3.2 Testing for sample symmetry

Another question could be, whether the data satisfy a specific sample symmetry $\dot{G}$ or only a lower sample symmetry $\dot{G}' \subset \dot{G}$. Thus we get the test problem:

$$H_0 : \mathit{ODF} \in \mathit{ExpRot}[L, \overset{\vdots}{G}, \dot{G}; \cdot] \quad vs. \quad H_1 : \mathit{ODF} \in \mathit{ExpRot}[L, \overset{\vdots}{G}, \dot{G}'; \cdot]$$

As before the likelihood ratio test can be used, because the hypothesis H_0 is a true sub-model of the alternative H_1.

3.3 Testing for specific potential functions

If we presume that in a specific sample the distribution of crystal orientations is governed by an energy function depending linearly on a single or several anisotropic physical properties $f_i(g)$, which are functions of low order harmonics, we can test for compatibility of the data with this hypothesis against a full $\mathit{ExpRot}[L, \overset{\vdots}{G}, \dot{G}; \cdot]$ family.

$$f_i(g) = \sum_{\tau \in I(L)} \theta_\tau^{(i)} \overset{\therefore}{T}_\tau(g) \tag{9}$$

The likelihood ratio test is appropriate for the resulting test problem:

$$\begin{aligned} &H_0 : \mathit{ODF} \in \left\{ \mathit{ExpRot}[L, \overset{\vdots}{G}, \dot{G}; \theta] : \theta = \textstyle\sum_i \alpha_i \theta^{(i)} \right\} \quad vs. \\ &H_1 : \mathit{ODF} \in \mathit{ExpRot}[L, \overset{\vdots}{G}, \dot{G}; \cdot] \end{aligned}$$

4 Regression for orientations

Up to now we have generally assumed that all observed orientations came from the same generating distribution. But more relevant are statistics for comparison of different textures. This can be a two sample experiment, after which we want to compare the textures under two different treatments. Or in case of multiple samples it could be interesting how texture depends on a process parameter. Possible models and tests for both situations are given here derived from a multivariate generalisation of the theory of generalized linear models with canonical link functions (MacCullagh & Nelder 1983).

4.1 The full regression model

In the most simple regression situation we deal with one real valued process parameter x. For each value of x the process will produce a certain texture. The most simple model for the influence of x on the texture is that x influences the parameter θ of the ODF linear:

$$\begin{aligned} &H_0 : \mathit{ODF}_x = \mathit{ExpRot}[L, \overset{\vdots}{G}, \dot{G}; \theta_0], \ \theta_0 \in \mathbb{R}^{I(L)} \quad vs. \\ &H_1 : \mathit{ODF}_x = \mathit{ExpRot}[L, \overset{\vdots}{G}, \dot{G}; \theta_0 + x\theta_x], \ \theta_0, \theta_x \in \mathbb{R}^{I(L)} \end{aligned}$$

Here ODF_x denotes the ODF generated under condition x. Other more sophisticated kinds of influence are possible. As long as the relation is a linear combination of θ, the joint distribution of all results of the experiments is a regular exponential family, and therefore the maximum likelihood estimator and the likelihood ratio test can be used as usual.

4.2 Two sample tests

As a special case of the regression model we can ask the question, whether two samples are equal or not, and if they are not equal how strong their departure is. We just have to introduce an artifical regression variable x taking the value 0 for one sample and the value 1 for the other sample. H_0 from the regression model is the hypothesis that both samples are equal, and H_1 is the alternative that both samples are not equal. The estimate of θ_1 tells something about the type and strength of departure.

5 ODF by grains and by volume

The procedures in this paper are concerned with the orientation distribution of the typical grain. Therefore the estimators in this paper say something about the ODF of the grains and not about the ODF of the typical bit of volume. Under the assumption that the texture does not depend on the size of the grain, both definitions of the ODF are equal and the grain-wise estimators are more precise, because they are not disturbed by the variation of grain size. If the probability for a grain to belong to the sample is proportional to its size, we observe a sample of grains which have the volume ODF as underlying distribution and therefore we can use the procedures in this paper for the volume ODF. This happens, if we measure the orientations on a sparse grid, such that we do not hit any grain twice and all measured grains have independent orientations. If our grid is sufficiently fine to measure the area of grains, and we want to model the dependence of the texture on the grain size we have to use spatial models as introduced in "Spatial Statistics for individual orientation measurements". If we presume dependence but do not want to model it, we should use some modified procedures, which are not given here.

6 References

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