SPATIAL STATISTICS FOR INDIVIDUAL ORIENTATION MEASUREMENTS

Spatial statistics for orientations

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Abstract

Individual orientation measurements do not only provide crystal orientations but also their spatial locations. This information can be used to analyse and describe the interaction of the orientated grains. This paper gives an outline of a statistical framework, in which processes of dependent crystal orientation can be modelled, simulated, and analysed. This contains a distribution model derived from the theory of Markov random fields and the theory of conditionally specified distributions. Pitfalls and possibilities of the simpler approach by the method of moments are discussed briefly.

Keywords: statistics, spatial statistics, individual orientation measurements, measurement error, texture models

1 Motivation

In many cases the orientation of an individual crystal grain is not independent of the orientation of its neighbours. This dependence actually effects any inference on these type of data in at least three ways. First, this behaviour violates the implicit assumption of independence, which is essential for all statistical inference on the measured data. Thus, adjusted statistical procedures for textures with dependent grain orientations are required. Secondly, this interdependence is an interesting phenomenon by itself, which should be incorporated into the representation of the texture. Thirdly, simulated textures should incorporate this dependence, too.

2 Distributions for spatial orientation processes

A large class of distributions for spatial stochastic processes representing regionalized crystal orientations can be derived from the theory of Markov random field (Cressie 1993) and conditionally specified exponential families (Arnold et al. 1991). This class is based on the class of distributions $ExpRot[L, \overset{:}{G}, \dot{G}; (\theta_\tau)_{\tau \in \overset{\therefore}{I}(L)}]$ 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 θ_τ, $\tau \in \overset{\therefore}{I}(L)$, by its distributional density:

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

Details on this family are given in the paper "Statistics for individual orientation measurements".

The central idea of the spatial model is that the conditional distribution of the crystallographic orientation of every grain given the orientation of the neighbouring grains has this distributional form. In mathematical terms, with M the set of grains:

$$P(g_i | g_j, j \in M \setminus \{i\}) = ExpRot[L, \overset{:}{G}, \dot{G}; \theta(g_j, j \in M \setminus \{i\})] \qquad \textbf{(1)}$$

For simplification we may assume pairwise interaction only. Then it follows by the theory of conditionally specified exponential families given in (Arnold et al. 1991) that the joint distribution density for the crystallographic orientations of all grains is:

$$\begin{aligned} f(g_i, i \in M) &= A(\alpha, \beta) * \\ &* \exp\left(\sum_{i \in M} \sum_{\tau \in \overset{\therefore}{I}(L)} \alpha_{\tau i} \, \overset{\therefore}{T}_\tau(g_i) + \sum_{\{i,j\} \subset M} \sum_{\tau \in \overset{\therefore}{I}(L)} \sum_{\sigma \in \overset{\therefore}{I}(L)} \beta_{ij\tau\sigma} \, \overset{\therefore}{T}_\tau(g_i) \, \overset{\therefore}{T}_\sigma(g_j) \right) \end{aligned} \qquad \textbf{(2)}$$

The parameters α_i and β_{ij} should be modelled as linear combinations of entities depending on the grain's shape and the relative position of the two grains i, j. Then the entire model is again an exponential family, and we can use methods known from the theory of exponential families. This could be the maximum likelihood estimation using a Metropolis like stochastic gradient algorithm proposed by L. Younes (Guyon 1995 p.221), and the likelihood ratio tests (under some additional assumptions) for the comparison of two models. Given a specified microstructure in form of a set of grains and known parameters α, β the texture can be simulated by a Metropolis algorithm (Guyon 1995). The details of estimation, test and simulation procedures are far beyond the scope of a six page introductory contribution. Generalisations to more complex dependence structures in various ways are available using the more general results of (Arnold et al. 1991), and using curved exponential families (Kass 1989).

Modelling of a simple dependence structure is exemplified by the following settings:

$$\alpha_{i\tau} = \theta_\tau^{(0)} * \text{"size of grain } i\text{"} * \theta_\tau^{(1)} \tag{3}$$

$$\beta_{ij\tau\sigma} = \theta^{(3)} * \text{"size of common boundary of grain } i \text{ and grain } j\text{"} * \gamma_{\tau\sigma} \tag{4}$$

with a γ such that:

$$\sum_\sigma \sum_\tau \gamma_{\tau\sigma} \dot{\ddot{T}}_\sigma(g_1)\, \dot{\ddot{T}}_\tau(g_2) \approx \begin{cases} 1, & g_1 \approx g_2 \; mod \, \dot{\ddot{G}} \\ 0, & else \end{cases} \tag{5}$$

representing a texture with preferred orientation ($\theta^{(0)}$) which depends on the grain size ($\theta^{(1)}$), and is affected by excessive small angle grain boundaries ($\theta^{(3)}$).

Similar to the effect of the grain size other characteristics of the grain could be incorporated into the model. These could be a Minkowski measure of the shape or an aspect of the location of the grain in the sample in case of inhomogeneous material.

3 Canonical statistics

For every exponential family model, there exists a set of associated canonical minimal sufficient statistics, which are unique up to affine linear transformation. These statistics contain as much information of the result of the experiment as required for parameter estimation or tests within the model. It is very interesting what these statistics are in the spatial model proposed here:

As an example we will us the model given by the equations (2),(3), and a more general model for the interaction term β:

$$\beta_{ij\tau\sigma} = \theta_{\tau\sigma}^{(3)} * \text{"size of common boundary of grain } i \text{ and grain } j\text{"} * \gamma_{\tau\sigma} \tag{6}$$

The canonical statistics associated with the parameters $\theta_\tau^{(0)}$ are the empirical means of low order harmonics:

$$\hat{C}_\tau = \hat{C}_l^{\mu\nu} = \sum_{i=1}^n \dot{\ddot{T}}_l^{\mu\nu}(g_i) \tag{7}$$

The canonical statistics associated with the parameters $\theta_\tau^{(1)}$ are the empirical means of low order harmonics weighted with the grain size:

$$\hat{\tilde{C}}_\tau = \hat{C}_l^{\mu\nu} = \sum_{i=1}^n (\dot{\ddot{T}}_l^{\mu\nu}(g_i) * \text{"size of grain } i\text{"}) \tag{8}$$

The canonical statistics associated with the interaction terms $\theta_{\tau\sigma}^{(3)}$ are some weighted non centered moments:

$$K_{\tau\sigma} = \sum_{i=1}^{n} \sum_{j \neq i} \ddot{T}_{\tau}(g_i)\, \ddot{T}_{\sigma}(g_j) * \text{"size of boundary } i, j\text{"} \qquad \textbf{(9)}$$

Because of a stereological argument for the measurement the volume of the grain can be replaced by it's visible area, and the area of the common boundaries can be replaced by their visible length.

4 Method of moments

4.1 Standard errors for harmonic coefficients

The model-driven approaches mentioned in the beginning of this contribution yield standard errors for the experimental harmonic coefficients of the ODF. An alternative approach could be to use the sample variance of the $\ddot{T}_l^{\mu\nu}(g_i)$, and divide it by n as usual:

$$\widehat{Var}(\hat{C}_l^{\mu\nu}) \stackrel{?}{=} \frac{1}{n(n-1)} \sum_{i=0}^{n} (\ddot{T}_l^{\mu\nu}(g_i) - \hat{C}_l^{\mu\nu})^2 \qquad \textbf{(10)}$$

However, that is not too splendid an idea, because this estimator is heavily biased and not consistent, if the orientation of grains is correlated. This problem has been discussed in depth in the context of regionalized random variables and kriging for univariate measurements cf. (Cressie 1993).

4.2 Simple inference with multiple samples

A simple workaround for this problem is to take multiple samples of equal size sufficiently far from each other that they can be assumed independent. Then we can replace the individual observed $\ddot{T}_l^{\mu\nu}(g_i)$ with the means of this statistic in each of the individual samples. Then we estimate the variance of the sample means. The overall mean is given by the mean of the sample means.

$$\hat{C}_l^{\mu\nu} = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{N(i)} \sum_{j=1} N(i)\, \ddot{T}_l^{\mu\nu}(g_{ij}) \qquad \textbf{(11)}$$

Here g_{ij} denotes the orientation of the grain j in sample i. The estimated variance of the overall mean can be calculated from the empirical variance of the sample means.

$$\widehat{Var}\hat{C}_l^{\mu\nu} = \frac{1}{n(n-1)} \sum_{i=1}^{n} \left(\frac{1}{N(i)} \sum_{j=1} N(i)\, \ddot{T}_l^{\mu\nu}(g_{ij}) - \hat{C}_l^{\mu\nu} \right)^2 \qquad \textbf{(12)}$$

Since these sample means are mean values, they are distributed approximately normal. Therefore statistical methods assuming multivariate normality such as cluster analysis, discriminant analysis, and MANOVA apply. The first two may have interesting applications in geology, where we may want to classify the unknown process from the observed texture. MANOVA or more general linear models may have interesting applications in materials sciences where we want to model the texture depending on the generating process described by a set of independent variables. Within the context of MANOVA random effects may be used to model the variation between different specimen, while fixed effects could be applied to model the influence of process parameters; MANOVA interaction terms may be used to model the interaction of the effects of process parameters.

Especially the question whether the textures of two objects are equal or not can be formulated as a test problem in the MANOVA context, since two textures, compatible with the same model M, are equal if and only if the sample means of the minimal sufficient statistics of M have the same mean in both objects. This is a multi-response heteroscedastic MANOVA model for the sample means of the minimal sufficient statistics of M as dependent variables and with a single dichotomic variable representing the object as independent variable.

5 Conclusion

Application of spatial statistics to individual orientation measurement data is possible and offers a broad variety of statistical procedures useful to answer many different questions about the observed texture of the investigated material. Only very few of them have been mentioned; many more can be developed in analogy to statistical procedures known for other localised data. There are many different tools for many different purposes available – what kind of purposes are we most interested in?

6 References

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