Approximation of Unmeasured Pole-Figures by Geostatistical Techniques

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1. Abstract

Our aim is to give a novel geostatistically based technique to recover any required complete pole figure, which was not at all or only incompletely measured, from a collection of measured diffraction data and to provide a local measure of precision for the reconstruction. The basic idea is to model the true orientation density, which is a function on the orientation group SO(3)/G, as a random field $f(g)$ with known mean 1. The measured diffraction intensities P(h,r) are mean values of $f(g)$ along geodesic fibers $B(h,r) = \{g : gh = r\}$ or corresponding tube shaped blocks in the domain of the random field. We propose a kind of block kriging to interpolate to unmeasured P(h,r). The method surpasses other methods in simplicity and generality with respect to the universatility of input data. It also allows to reconstruct local portions of pole figures from incomplete measurements and gives the kriging error as a measure of precision.

2. Introduction

The texture of crystalline material, i.e., the orientation distribution of crystal lattices, provides insight into the deformation history and deformation mechanisms of ductile deformed rocks and minerals. During deformation in different heat and pressure conditions, different deformation mechanisms are activated and thus different textures evolve. Various techniques of texture measurements are available. The most traditional one is the measurement of the intensities of x-ray diffraction by specified lattice plane h (e.g. 110, 120, 111) in all possible directions r of the sample. The result, called pole-figure, is an intensity for each direction of the axial directional sphere. These intensities are typically plotted in a Schmidt net and can be interpreted by those who are familiar with texture analysis. However, typically only a few pole-figures are actually measured while others (e.g. 001) might be more informative. Due to time limitations and the geometry of the measurement process even these are measured only partially, giving a collection of intensity measurements locally unevenly distributed over the different pole figures. Measurements are integrated intensities over area patches of the corresponding ideal pole figures. Various techniques are available to reconstruct an orientation distribution from Polefigures (see Bunge 1983, Schaeben 1993).

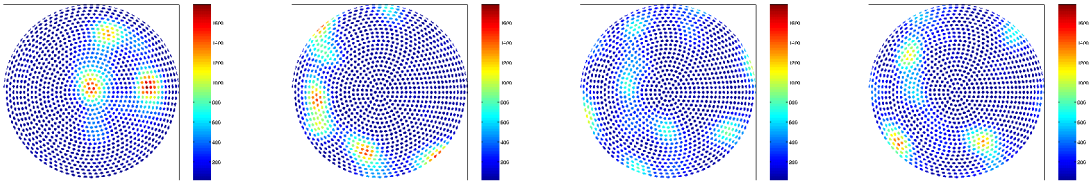

Fig. 1. Simulated polefigure measurements {102}, {110}, {111}, and {021} used for the reconstruction

3. Geostatistical Modeling of ODFs

The basic idea of this paper is to view the unknown ODF as a random field $f(g)$ on a curved surface. The locations are orientations of a crystall in a space $g \in SO(3)/G$, where $SO(3)$ denotes the Special Orthogonal group of 3 dimensions (i.e. the group of rotations) and G denotes the rotation part of the Laue group of the crystal. We assume second order stationarity under rotation (c.f. Moritz 1977):

$$E[f(g)]E[f(g')], \quad c(g,g') = \mathrm{cov}(f(g), f(g')) = \mathrm{cov}(f(\sigma g), f(\sigma g')), \sigma \in SO(3)$$

On one hand this covariance can be seen as a covariance of a subjective probability given by our lack of knowledge about the ODF $f(g)$ on the other hand it can be seen as some prior information on roughness of the ODF. In both views it can be estimated from the data.

Every realisation of the field f is a probability density function, which implies that its mean over $SO(3)/G$ is the total probability 1. Thus due to stationarity its expectation for any fixed g is also 1:

$$\forall g : E[f(g)] = 1$$

4. Geostatistical Modeling of ODFs, X-Rays and Detectors

The problem is that unlike in geostatistics we can not actually measure values of the ODF at specific orientations. The texture of a whole specimen can only be measured indirectly, by diffraction measurements: The specimen is exposed to a directed beam of some (typically monochromatic) wave (e.g. X-rays or neutrons). The wave is “reflected” by lattice planes with a specific relation of inter plane spacing and the wavelength of the beam and then detected by a particle counting (photons or neutrons) detector, which is located the position where plane of a specific spatial orientation would reflect the beam to. Since in general the inter plane spacing of different lattice planes are different only one plane (e.g. {021}) will be in reflection position for a given wavelength and geometry. The density of lattice planes h beeing in a given reflection direction r is denoted by $P_h(r)$. It is the integral over all parts of the ODF with gh = r or gh =-r. Classically this relation is written as (Bunge 1982):

$$P_h(r) = \int_{\{gh=\pm r\}} f(g)dg$$

The set {gh = ±r} corresponds to two disjunctive (great) circles on the sphere like group SO(3) (Schaeben 1993). The integration is thus along this circular lines. Since the detector has some extend, it detects the beam for a small (typically circular) area patches A (e.g. A = {r: (r, r_0) > cos(1°)}) of directions r.

$$P_h(A) = \int_{\{\pm gh \in A\}} f(g)dg$$

Thus the true integration area corresponds to two thin tubes on SO(3) and can be seen as integrals over blocks leading us to a situation of Block Kriging (c.f. Cressie 1993) with some very long thin blocks $B_i = \{\pm gh \in A_i\}$. The integration is with respect to the Haar measure of $SO(3)$ given in Euler angels by (Bunge 1982) $dg = \frac{1}{4\pi^2}\sin\Phi d\phi_1 d\Phi d\phi_2$. Since the intensities are measured by counts I_i in a certain block A_i of randomly reflected (quantum) particles the actual measurement has a Poisson distributed counting error:

$$I_i \sim \text{Poisson}\,(a_i P_{h_i}(A_i) + b_i),$$

with a factor a_i depending on the beam intenstity, the reflectivity of the lattice plane, the easurement angle, the irradiation time and so on and a background b_i, such that we can use

$$z_i = \frac{I_i - b_i}{a_i}$$

as a measurement of $P_{h_i}(A_i)$. The Poisson error of I_i induces for z_i a nugget variance of

$$\sigma_i^2 = \frac{a_i P_{h_i}(A_i) + b}{a_i^2} = \frac{P_{h_i}(A_i)}{a_i} + \frac{b}{a_i^2}$$

Clearly the measurement error σ^2_i depends on the unknown $P_{hi}(A_i)$. However we can use the measurement z_i as first approximation and later replace it by a kriging prediction of the value for a second iteration.

5. Modeling the Covariogram

With respect to valid covariance models we need to take care of several specialties of the specific domain our "random field" is defined on

• *Different understanding of stationarity and isotropy on* $SO(3)$

For simplicity we propose to assume that for a triclinic texture the covariance only depends on the angular difference of the orientations g_i and g_j:

$$c(g_i, g_j) = \text{cov}(f(g_i), f(g_j)) = k(\angle g_i g_j^{-1}).$$

• *Positive semidefinitness on noneuclidean space*

Unlike the classical situation we cannot check positive definiteness by an Euclidean version of Bochners theorem (c.f. Cressie 1993), since the space is not Euclidean. However a similar theorem holds here (c.f. Boogaart et al. 2005)

Theorem: $c(g_i, g_j)$ is positive semidefinite if and only if $a_l \geq 0$ for all l in

$$k(\omega) = \sum_{l=0}^{\infty} a_i U_{2l}(\cos\frac{\omega}{2})$$

Some of the known distribution density models on $SO(3)$ such as Fisher-Matrix-Distribution and

Brownian distribution (Schaeben&Boogaart 2003) have this property. Every isotropic covariance model $c(h)$ valid in R^9 can be used, by setting $h = \|g_i - g_j\|$ with the orientations g_i and g_j represented as matrices and $\|\cdot\|$ defined by the square root of the sum of the squares of the elements of the matrix. Let us call the selected kernel $k_{bw}(\omega)$, where bw denotes the bandwidth-parameter. Fornow $k_{bw}(\omega)$ is assumed to be normalized as a probability density function.

• *The sum 1 constraint of probability density functions*

We are estimating a probability density function and thus know that

$$0 = \mathrm{var}(1) = \mathrm{var}(\mathrm{P}(SO(3))) = \mathrm{var}(\int_{SO(3)} f(g)dg) = \int_{SO(3)} \int_{SO(3)} c(\angle g_i g_j^{-1}) dg_i dg_j$$

Using harmonic expansions one can show that

$$\int_{SO(3)} \int_{SO(3)} c(g_i g_j) dg_i dg_j = \int_{SO(3)} \int_{SO(3)} k(\angle g_i g_j^{-1}) dg_i dg_j = \int_{SO(3)} k(\angle g) dg = a_0$$

implying $a_0 = 0$. This is not true for any of the known kernels $k_{bw}(\omega)$, since due to the normalization as probability density function we always have $\int k_{bw}(\omega)\mathrm{dg} = 1$. However we can always use $k_{bw}(\omega) - 1$ instead.

• *Crystal symmetry*

For non triclinic materials the texture is symmetric with respect to a symmetry group G:

$$\forall g \forall \sigma \in : f(g) = f(g\sigma)$$

This can be achieved by symmetrizing any triclinic ODF f_0 with the symmetry group:

$$f(g) = \frac{1}{|G|} \sum_{\sigma \in G} f_0(g\sigma)$$

Correspondingly if f_0 has a covariogram c_0 we get

$$c(g_i, g_j) = \mathrm{cov}(f(g_i), g(g_j)) = \frac{1}{|G|^2} \sum_{r \in G} \sum_{\sigma \in G} c_0(g_i\sigma, g_j r) = \frac{1}{|G|} \sum_{\sigma \in G} c_0(g_i\sigma, g_j)$$

Summarizing we get an adequate covariance model by taking:

$$c(g_i, g_j) = \frac{sill}{|G|} \sum_{\sigma \in G} \frac{k_{bw}(\angle g_i \sigma g_j) - 1}{k_{bw}(0) - 1}$$

Where we have a range like parameter bw and a sill parameter. Introduction of a nugget effect is useless since we are using Block-Kriging. Several shapes can be selected by choosing one of the known families for k_{bw}.

6. Estimation of the Covariogram

Since no individual values of $f(g)$ are observed we have to estimate the covariance from the integral measurements. Covariance of these measurements is given according to the theory of block kriging (c.f. Cressie 1993) by

$$c_{ij} := \mathrm{cov}(z_i, z_j) = \int_{A_i}\int_{A_j} c(g_i, g_j)dg_i dg_j + \delta_{ij}\sigma_i^2$$

which typically needs to be calculated numerically. Some analytical solutions can be found in (Boogaart et al. 2005). If the data is concentrated to some polefigures, we can compute covariograms and crosscovariograms of measurements in different polefigures (Fig. 2), otherwise the empirical and model covariance matrix must be fitted directly.

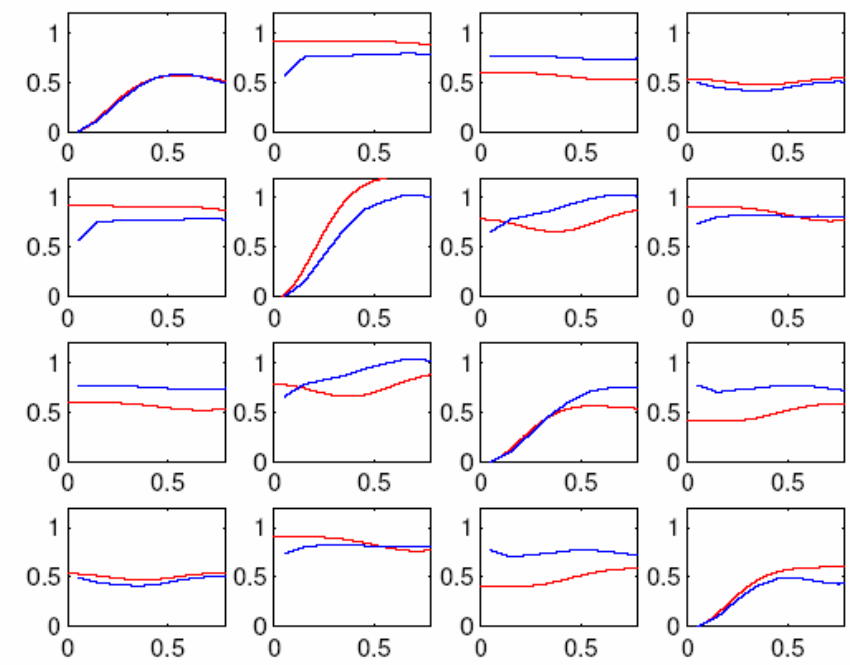

Fig. 2. Emperical (blue) and fitted (red) (cross-)variograms of the pole figure datasets

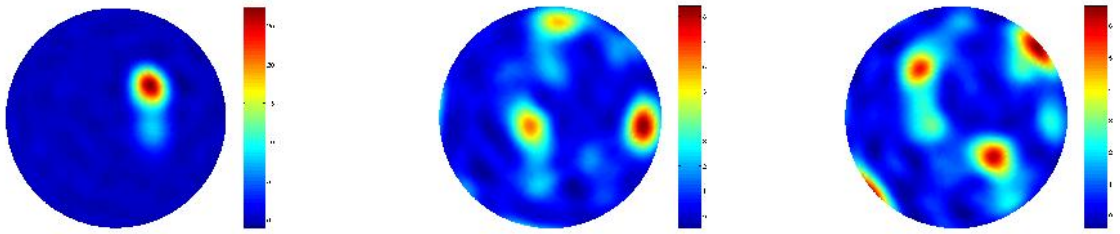

Fig. 3. Reconstructed polefigures {102}, {110}, and {111} of our simulated dataset.

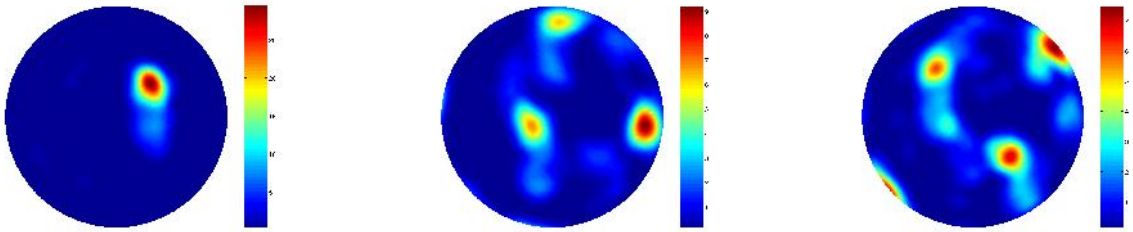

Fig. 4. True polefigures {001}, {101} and {011} of our simulated dataset. These polefigures cannot be measured directly

7. Block Kriging Applied to Polefigures

Again with the arguments of Block Kriging the covariance of the observations with a pole intensity $P_h(r)$ to be estimated is given by:

$$c_i := \operatorname{cov}(z_i, P_h(r)) = \int_{A_i} \int_{\{gh=\pm r\}} \operatorname{cov}(f(g_i), f(g_j)) dg_i dg_j$$

The kriging estimate is than given by simple block kriging with mean 1:

$$\hat{P}_h(r) := 1 + \begin{pmatrix} z_1 - 1 \\ \mathbf{j} \\ z_n - 1 \end{pmatrix}^t \begin{pmatrix} c_{11} & \mathbf{h} & c_{1n} \\ \mathbf{j} & \mathbf{l} & \mathbf{j} \\ c_{n1} & \mathbf{i} & c_{nn} \end{pmatrix}^{-1} \begin{pmatrix} c_1 \\ \mathbf{j} \\ c_n \end{pmatrix}$$

8. Conclusions

Kriging can be used for tasks that in a first place do not look like geostatistics at all. The assertion that additional polefigures can only be calculated by an intermediate step of estimating an ODF is falsified by this method (c.f. Matthies&Esling 1998). Problems with the odd harmonics are not relevant since pole figures i.e. the data and the reconstruction only use the even harmonic parts.

9. References

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