

PDF-to-ODF Inversion by Approximation with Spherical Radial Basis Functions

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Abstract. The radial basis function method is applied to reconstruct the orientation density function and the pole density function from any arbitrary set of X-ray intensities. The mathematical foundations are given as well as numerical results.

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Introduction

The analysis of crystallographic preferred orientations by means of orientation density functions and pole density functions is a widely used method in texture analysis (cf. Bunge [4], Matthies et. all [8]). On the other hand, the radial basis function method (cf. Hubert [7]) or kriging method with covariance functions (cf. Wahba [11]) has already found its way into many fields of application. Utilizing the radial basis function method to interpolate X-ray intensities and to reconstruct the orientation density function of a specimen we introduce a new method in addition to hitherto used harmonic method (cf. Bunge [4]), maximum entropy (Matthies et. all [8], Schaeben [9]) or component fit method (cf. Helming, Eschner [6]). The main advantage of the radial basis function method is that it can deal with X-ray intensities that are measured for arbitrary arranged crystal and specimen directions. In particular the method is not restricted to data that are measured in pole figure notation, i.e. for a few crystal directions and many specimen directions.

We consider a polycrystalline specimen consisting of crystals associated to a certain *point group* $G \subseteq SO(3)$. Each crystal provides a canonical crystal coordinate system which is well defined up to action of the point group G . Fixing a specimen coordinate system we define the *orientation* of a crystal to be the rotation $g \in SO(3)/G$ that realizes the basis transformation from the crystal coordinate system to the specimen coordinate system. Directions relative to the

crystal coordinate system we will call *crystal directions* and directions relative to the specimen coordinate system *specimen directions*.

The *orientation density function* (ODF) $f: \text{SO}(3)/G \rightarrow \mathbb{R}$ is defined as the relative frequency of orientations by volume within a specimen, whereas the *pole density function* (PDF) $P: \text{S}^2/G \times \text{S}^2 \rightarrow \mathbb{R}$ is defined as the relative frequency $P(h, r)$ of orientations $g \in \text{SO}(3)/G$ rotating the crystal direction $h \in \text{S}^2/G$ onto the specimen direction $r \in \text{S}^2$. The ODF f and the PDF P of a specimen are connected by the crystallographic X-ray transform on $\text{SO}(3)/G$ (cf. Bunge [4, Section 4.2])

$$\mathcal{R}f(h, r) := \int_{\{g \in \text{SO}(3)/G \mid r \in gh\}} f(g) dg, \quad (h \in \text{S}^2/G, r \in \text{S}^2), \quad (1)$$

$$P(h, r) = \mathcal{X}f(h, r) := \frac{1}{2} (\mathcal{R}f(h, r) + \mathcal{R}f(-h, r)). \quad (2)$$

For a fixed crystal direction $h \in \text{S}^2/G$ the PDF $P(h, \cdot): \text{S}^2 \rightarrow \mathbb{R}$ is called *pole figure*. Conversely, fixing specimen directions $r \in \text{S}^2$ we obtain *inverse pole figures* $P(\cdot, r)$ which are of great importance for many physical properties.

There are several experiments like X-ray and neutron synchrotron diffraction that allow to measure the PDF of a specimen for a sequence of crystal and specimen directions. To such a list of PDF measurements $(P_i)_{i=1}^N$ with respect to crystal and specimen directions $(h_i, r_i)_{i=1}^N$ we refer as to a *set of X-ray intensities* $(P_i, h_i, r_i)_{i=1}^N$. It is a central problem in texture analysis to reconstruct the original PDF P and the original ODF f from a set of X-ray intensities. Since both, ODF and PDF, are not uniquely determined by the data set we have to make additional assumptions to obtain approximations \tilde{f} resp. \tilde{P} of the original density functions.

The general idea of the radial basis function method

First of all it should be noted that the spherical X-ray transform maps all odd generalized spherical harmonics onto zero. This implies that beside the none negativity property there is no chance to determine the odd part of an ODF from its X-ray transform. Therefore the PDF-to-ODF reconstruction problem on the basis of the pole figure intensities $(P_i, h_i, r_i)_{i=1}^N$ can be split into

1. Estimation of the even part \tilde{f}_e of the true ODF f such that $\mathcal{X}\tilde{f}_e(h_i, r_i) \approx P_i$ for all $i = 1, \dots, N$.
2. Estimation of the odd part \tilde{f}_o of the true ODF f such that $\tilde{f}_e + \tilde{f}_o \geq 0$.

We will deal in this paper with the first step only. For the second step the reader is referred to Boehlke [1].

In order to find a method to determine the even part \tilde{f}_e we start our consideration with a simple example. Assume we just measured the X-ray intensity P_1 in a single point, i.e. for a pair (h_1, r_1) of crystal and specimen directions. Then we know that the integral of \tilde{f}_e over all rotations $C(h_1, r_1)$ that map the crystal direction h_1 onto the specimen direction r_1 equals P_1 . Clearly there are arbitrary many ODF that yield this property. However, in the absence of additional knowledge one should prefer an ODF that is uniformly distributed along the fibre $C(h_1, r_1)$. Mathematically it is characterized by maximum entropy or minimum information. Hence a suitable estimate is a fibre symmetric ODF the concentration of which corresponds to the expected smoothness of the true ODF.

This observation can be generalized to a concept for estimation of the even part of an ODF from an arbitrary set of corresponding X-ray intensities (P_i, h_i, r_i) . For each measured intensity

P_i with respect to the directions (h_i, r_i) we generate an even fiber symmetric function F_{h_i, r_i} with center in $C(h_i, r_i)$ and zero integral. Now we make the ansatz

$$\tilde{f}_e(g) = 1 + \sum_{i=1}^N c_i F_{h_i, r_i}(g), \quad (g \in \text{SO}(3)) \quad (3)$$

and calculate the coefficients (c_i) such that the X-ray transform of \tilde{f}_e approximates the pole intensities. In the ansatz (3) we have added the uniformly distributed ODF 1 in order to observe the constraint that ODF has always integral one.

There are two equivalent general concepts leading to representation formula (3) of the best estimate for f_e too. The first concept is called radial basis function method and is studied in various applications. The central idea of the radial basis function method is to specify the inversion problem as the minimizing problem to find an ODF that fits best to the pole intensities and is maximum smooth. Here smooth means that a certain Sobolev norm is small. If the domain of the minimizing problem equipped with this norm provides a reproducing kernel Hilbert space structure one can show that the solution of the minimizing problem is of form (3). Moreover it follows the existence of coefficients (c_i) such that the interpolation property is fulfilled. For a detailed presentation of these arguments the reader is referred to [3]. The second equivalent approach is given by the kriging method with covariance function which minimizes the the estimated error. The equivalence of the kriging and the radial basis function method is shown for example in Wahba [2].

Determination of the even part

Let us now determine the coefficients (c_i) explicitly. We start with a set of X-ray intensities (P_i, h_i, r_i) and a fibre-symmetric kernel $F_{h, r}(g)$ on $\text{SO}(3)$ with zero integral. The X-ray transform of \tilde{f}_e in equation (3) is given by

$$\mathcal{X}\tilde{f}_e(h, r) = 1 + \sum_{i=1}^N c_i \mathcal{X}F_{h_i, r_i}(h, r), \quad (4)$$

where c is the vector $(c_i)_{i=1}^N$ and M denotes the Gram matrix

$$M = \begin{pmatrix} \mathcal{X}F_{h_1, r_1}(h_1, r_1) & \mathcal{X}F_{h_2, r_2}(h_1, r_1) & \cdots & \mathcal{X}F_{h_N, r_N}(h_1, r_1) \\ \mathcal{X}F_{h_1, r_1}(h_2, r_2) & \mathcal{X}F_{h_2, r_2}(h_2, r_2) & \cdots & \mathcal{X}F_{h_N, r_N}(h_2, r_2) \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{X}F_{h_1, r_1}(h_N, r_N) & \mathcal{X}F_{h_2, r_2}(h_N, r_N) & \cdots & \mathcal{X}F_{h_N, r_N}(h_N, r_N) \end{pmatrix}. \quad (5)$$

Let $P = (P_i)_{i=1}^N$ and $e_1 = (1, \dots, 1) \in \mathbb{R}^N$. Then the solution of the interpolation problem $\mathcal{X}f(h_i, r_i) = P_i$ is given by the solution by the system of linear equations

$$Mc = P - e_1.$$

However, in practice the measured X-ray intensities (P_i) are in general effected by random noise. Therefore it is more appropate to look for a function that does not exactly interpolate the data points but is a compromise between fitting the data and being maximum smooth. Such a function is obtained as the solution of the regularized system of linear equations

$$(M + \lambda \text{Id})c = P - e_1. \quad (6)$$

The regularization parameter $\lambda > 0$ determines the balance between fitting to the data and smoothness of the solution. In [3] it is shown that the system (6) has for all $\lambda > 0$ a well defined solution.

So far we have not considered crystal symmetries at all. However, they are not only necessary to obtain correct results, but also improve the accuracy of the calculation. Let $G \subseteq \text{SO}(3)$ be the point group of a crystal. Then

$$\ddot{F}(h, r) = \sum_{g \in G} F_{gh, r}, \quad (h, r \in \mathbb{S}^2)$$

defines a fibre symmetric ODF with respect to the crystal symmetry G . Replacing $F_{h, r}$ in (4) and (5) by \ddot{F} we obtain a method that allows for the crystal symmetry G .

Examples of fibre symmetric kernels

For the numerical work we are interested in fibre symmetric kernel functions F the Radon transform of which can be easily calculated. The fibre symmetric von Mises-Fischer distributed (or GAUSS-shaped, Matthies et. all [8]) kernel is given by

$$F_{h, r}(g) = \frac{\kappa}{\sinh(\kappa)} e^{\kappa(g h \cdot r)}, \quad (7)$$

where $\kappa \in \mathbb{R}_+$ is the concentration parameter. Denote I_n the modified Bessel function of first kind. Then the Radon transform of F is given by (cf. Matthies et. all [8])

$$\mathcal{R}F_{h_1, r_1}(h_2, r_2) = \frac{\kappa}{\sinh(\kappa)} I_0(\kappa \sin \omega_1 \sin \omega_2) e^{\kappa \cos \omega_1 \cos \omega_2}, \quad (8)$$

where we have set $\omega_1 = \angle h_1 h_2$ and $\omega_2 = \angle r_1 r_2$. In Figure 1 the Radon transformed fibre symmetric von Mises-Fischer kernel is plotted as a function in ω_1 and ω_2 . Since the calculation of the modified Bessel function is of remarkable computational effort we want to introduce a second kernel. Let $F_{h, r}$ be given by

$$F_{h, r}(g) = \ln \left(\frac{1 + \kappa}{1 - \kappa} \right)^{-1} \frac{2\kappa}{1 - 2\kappa(g h \cdot r) + \kappa^2}, \quad (9)$$

where $\kappa \in (0, 1)$ determines the concentration. This kernel is formally similar to the well known Abel-Poisson kernel. However, its Radon transform has the simple formula

$$\mathcal{R}F_{h_1, r_1}(h_2, r_2) = \ln \left(\frac{1 + \kappa}{1 - \kappa} \right)^{-1} \frac{2\kappa}{\sqrt{1 + \kappa^2 - 2\kappa \cos(\omega_1 - \omega_2)} \sqrt{1 + \kappa^2 - 2\kappa \cos(\omega_1 + \omega_2)}}, \quad (10)$$

with the same definitions for ω_1 and ω_2 as in (8). For a plot of $\mathcal{R}F$ as a function in ω_1 and ω_2 see Figure 1.

Numerical results

Now we are going to demonstrate the radial basis function method on a simple example. Let T be the cubical point group and let

$$K = \frac{B(3/2, 1/2)}{B(3/2, \kappa + 1/2)} \cos(\omega/2)^{2\kappa} \quad (11)$$

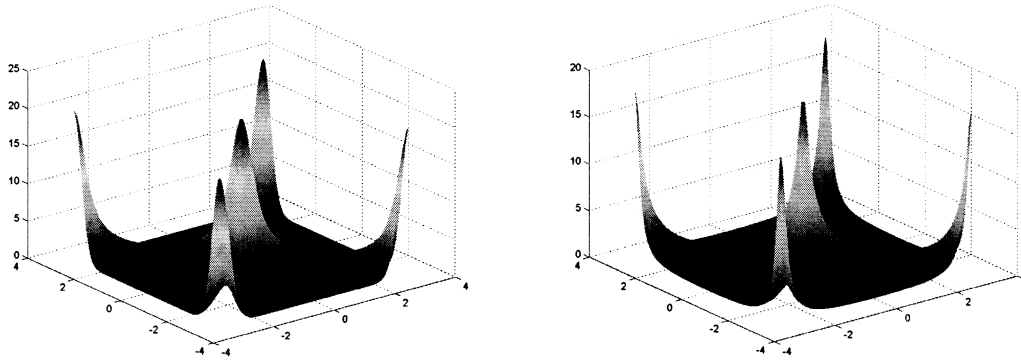


Fig. 1: The Radon transformed von Mises-Fischer kernel with parameter $\kappa = 10$ and the Radon transformed Square Singularity kernel with parameter $\kappa = 0.8$ as functions in ω_1 and ω_2 .

be the de la Vallée-Poussin kernel. The parameter κ describes the concentration of $K_{\text{SO}(3)}$. We define a cubic symmetric test ODF

$$f(g) = \sum_{i=1}^3 \lambda_i \sum_{\hat{g} \in T} K(g_i, g\hat{g}) \quad (12)$$

as the linear combination of three cubic symmetric de la Vallée-Poussin kernels, where the first component is centered in $g_1 = \text{Id}$ and has the parameter $\kappa_1 = 0.8$ and the two other components has centers in $g_{2/3} = (\pm 0.1, 0, 0)$ (Euler angles) respectively and parameter $\kappa_{2/3} = 0.9$. The coefficients are set to $\lambda_1 = 0.9$ and $\lambda_{2/3} = 0.05$. Hence the ODF \tilde{f} is nearly unimodal distributed with none radial symmetric peak in the identical rotation. Using the fact that

$$(\mathcal{R}K)(g, h, r) = (1 + \kappa) \cos\left(\frac{\angle(gh, r)}{2}\right)^{2\kappa} \quad (13)$$

the PDF of f can be easily calculated. In order to simulate a X-ray diffraction experiment we calculate the pole figures to the crystal directions $\{100\}$, $\{110\}$, $\{111\}$ and $\{221\}$ and a set of 180 approximately equidistant distributed specimen directions and adding to them some $\mathcal{N}(0, 0.05^2)$ -distributed noise. In Table 1 are listed the maximum-norm errors of the reconstructed ODF and PDF with respect to the fibre symmetric von Mises-Fischer and the Square Singularity kernel and different parameters.

kernel	parameter κ	$\ P - \tilde{P}\ _\infty$	$\ f_e - \tilde{f}_e\ _\infty$	$\ f - \tilde{f}\ _\infty$
Square Singularity	0.7	0.15	0.25	0.8
Square Singularity	0.8	0.15	0.35	0.8
fibre von Mises-Fischer	10	0.3	0.55	1.1
fibre von Mises-Fischer	20	0.15	0.25	0.7

Table 1: The maximum errors of the estimated PDF and ODF to f with respect to different kernels and the regularization parameter 0.05.

Conclusions and Outlook

We presented a method that allows to reconstruct the even part of an ODF from a set of X-ray intensities. The advantage of the method is that it can deal with X-ray intensities to arbitrary arranged crystal and specimen directions. Moreover, the solution is adapted to this arrangement in the sense that in regions where the crystal and specimen directions are dense the solution is effected by many kernel functions and therefore approximates more exactly then in regions of coarser measurements.

A second advantage of the radial basis function method is the simple numerical implementation. The problems reduces to solve a system of linear equations where the matrix is symmetric positive definite. In the special case that the grid (h_i, r_i) provides for each h a regular structure on S^2 the matrix even turns out to be of block Toeplitz structure.

A disadvantage of the presented method is that it does not observe the none negativity property of the PDF. However, the general approximation theorem of the radial basis function method implies that of negativity of the estimated PDF is bounded by a constant which becomes smaller when more X-ray intensities are measured.

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