Texture analysis of heterogeneous data—a farewell to *F*-coefficients

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Abstract

This contribution describes the mathematical and numerical possibility to analyse heterogeneous data, e.g. experimental intensity data measured for many crystallographic but few sample directions, adaptively refined high resolution intensity data, or a mixture of diffraction intensity data and individual orientation data from scanning electron microscopy.

These possibilities are put forward within the dual approach to texture analysis provided by the differential equation governing pole figures. The general solution of this differential equation is represented both in terms of spherical harmonics or characteristics. The resulting systems of equations are capable of considering such heterogeneous data as mentioned above.

The eventual aim of this contribution is to show that (i) the mostly tacit 'paradigm' of texture analysis that additional pole figures can be calculated from experimental pole figures only by using a detour via the ODF is not correct, and (ii) any function satisfying the differential equation governing pole figures is the actual pole figure projection, or X-ray transform, of a common function defined in a higher dimensional space.

Summarily, it is shown that the two dual approaches to texture analysis provided by the projection formula or the differential equation are equivalent, but put emphasis on different issues of the same problem. © 2000 Elsevier Science Ltd. All rights reserved.

1. Hyperspherical X-ray transforms, pole figures

The analysis of preferred crystallographic orientation is referred to as texture analysis. A probability density function $f(g)$ defined on the group SO(3) of rotations or a subset G of SO(3) depending on the crystal symmetry, respectively, is referred to as orientation density function (ODF) describing the distribution of crystallographic orientations by volume. While orientation density functions may be mathematically determined from individual orientation measurements directly in some applications, they are not generally directly accessible in many other applications. In these applications it is common practice to measure diffraction pole figures of a few crystallographic forms h. An introduction to texture analysis with special emphasis on geological applications is given by Wenk (1985).

A diffraction pole figure is mathematically represented as the projection of an orientation density function $f : \mathrm{SO}(3) \mapsto \mathrm{IR}_+^1$ basically provided by the integral operator

$$(\mathscr{P}_{\mathbf{h}}f)(\mathbf{r}) = \frac{1}{2\pi} \int_{\{g \in \mathrm{SO}(3) | \mathbf{h} = g\mathbf{r}\}} f(g)\, \mathrm{d}\, v(g) = P(\mathbf{h}, \mathbf{r}) \qquad (1)$$

where the function $P(\mathbf{h}, \mathbf{r})$: $S^2 \times S^2 \mapsto \mathrm{IR}_+^1$ for a given crystallographic direction $\mathbf{h} \in S^2 \subset \mathrm{IR}^3$ may be referred to as hyperspherical X-ray transform of f with respect to $\mathbf{h}$. The path of integration $\{g \in \mathrm{SO}(3) | \mathbf{h} = g\mathbf{r}\}$ in Eq. (1) is a circle restricted to the three-dimensional sphere $S^3 \subset \mathrm{IR}^4$ (Schaeben, 1996).

Next, for reasons originating in crystallography and Friedel's empirical law, which states that the diffracting X-ray cannot distinguish between top and bottom of the lattice planes, i.e. the directions $\mathbf{h}$ and $-\mathbf{h}$ cannot be distinguished in the diffraction experiment even if the crystal itself is not centrosymmetric, the basic crystallographic X-ray transform is defined as

$$(\tilde{P}_{\mathbf{h}}f)(\mathbf{r}) = \tfrac{1}{2}(P(\mathbf{h}, \mathbf{r}) + P(-\mathbf{h}, \mathbf{r})) = \tilde{P}(\mathbf{h}, \mathbf{r}) \qquad (2)$$

Now, obviously,

$$\tilde{P}(\mathbf{h}, \mathbf{r}) = \tilde{P}(-\mathbf{h}, \mathbf{r}) = \tilde{P}(\mathbf{h}, -\mathbf{r}) \qquad (3)$$

that is, $\tilde{P}$ is an even function in both arguments $\mathbf{h}, \mathbf{r} \in S^2$, and therefore the operator of Eq. (2) maps essentially from SO(3) (equivalent to S_+^4) onto the cross-product $S_+^2 \times S_+^2$ of two upper hemispheres, or equivalently from the projective space H^3 to the cross-product space $H^2 \times H^2$ of projective planes.

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For a crystallographic orientation density function $f \in C^2(\mathrm{SO}(3))$, its corresponding crystallographic h pole figure $\tilde{P}_\mathrm{h}$ of the crystal form $h = \{\mathbf{h}_m | m = 1, ..., M_\mathrm{h}\} \subset S^2$ of multiplicity M_h corresponding to crystal-symmetrically equivalent lattice planes $\{(hkl)_m | m = 1, ..., M_\mathrm{h}\} \subset \mathbb{Z}^3$ is defined for $\mathbf{r} \in S^2$ as

$$\tilde{P}_\mathrm{h}(\mathbf{r}) = (\tilde{P}_\mathrm{h}f)(\mathbf{r}) = \frac{1}{M_\mathrm{h}} \sum_{m=1}^{M_\mathrm{h}} P(\mathbf{h}_m, \mathbf{r}) \qquad (4)$$

such that

$$\int_{S^2_+} \tilde{P}_\mathrm{h}(\mathbf{r}) \, \mathrm{d}\, s(\mathbf{r}) = 1$$

when

$$\int_{\mathrm{SO}(3)} f(g) \, \mathrm{d}\, v(g) = 1$$

Summation in Eq. (4) is effectively over all directions $g_\mathrm{B}\mathbf{h}$, $-g_\mathrm{B}\mathbf{h}$, $g_\mathrm{B} \in G_\mathrm{B}$, which are symmetrically equivalent with respect to the associated Laue group $\tilde{\mathscr{G}}_\mathrm{B}$. Eventually,

$$(\tilde{P}_\mathrm{h}f)(\mathbf{r}) = \frac{1}{\#G_\mathrm{B}} \sum_{g_{\mathrm{B}_j} \in G_\mathrm{B}} \tilde{P}\!\left(g_{\mathrm{B}_j}\mathbf{h}, \mathbf{r}\right) = \tilde{P}(\mathbf{h}, \mathbf{r}) \qquad (5)$$

where h denotes the set of symmetrically equivalent cystallographic directions $\mathbf{h}_m$ related to each other by the associated Laue group, and $\mathbf{h}$ denotes an arbitrary element of h. Thus, $\tilde{P}_\mathrm{h}(\mathbf{r})$ and $\tilde{P}(\mathbf{h}, \mathbf{r})$ will no longer be distinguished.

In the past, main interest of texture analysis was focused on the inverse problem to find a reasonable orientation density function conforming with given intensity data corresponding to pole figures of some crystal forms. In a strict mathematical sense a general solution of this problem does not exist because crystallographic pole density functions provide too little information due to their evenness. However, for practical purposes several methods exist to resolve the problem in sensible ways. From a mathematical point of view, all known methods have some heuristics in common.

It was not appreciated that pole figures are rather complex mathematical entities governed by a differential equation of ultrahyperbolic or Darboux type, respectively. Conventional texture analysis did not pay any attention to this more sophisticated property; on the contrary, only recently it was declared as being useless (Matthies and Esling, 1998); however, their polemic is erroneous (cf. Nikolayev and Schaeben, 1999). Pursuing the approach by the differential equation governing spherical X-ray transforms provides the means (i) to construct a dual form of texture analysis and (ii) to establish a complete analogy to mathematical tomography.

2. The ultrahyperbolic differential equation of texture goniometry

The conventional notation $\tilde{P}_\mathrm{h}(\mathbf{r})$ of texture analysis was dropped in favour of $\tilde{P}(\mathbf{h}, \mathbf{r})$ to emphasize its features of a general axis probability density function ('allgemeine Achsenverteilungsfunktion' $\tilde{A}(\mathbf{h}, \mathbf{r})$, Bunge, 1982, p. 53) as follows.

Let Δ denote the Laplace–Beltrami operator, and assume $f \in C^2(\mathrm{SO}(3))$ and hence $P \in C^2(S^2 \times S^2)$. Then

$$(\Delta_\mathrm{h} - \Delta_\mathrm{r})P(\mathbf{h}, \mathbf{r}) = 0 \qquad (6)$$

where the equality is directly derived from the definition, Eq. (1) by simultaneously substituting $\mathbf{h},\mathbf{r},g$ by $\mathbf{r},\mathbf{h},g^{-1}$, and in particular without reference to harmonic functions and their properties. It is referred to as ultrahyperbolic differential equation in mathematical physics (cf. John, 1938; Courant and Hilbert, 1953), or Darboux partial differential equation in tomography (cf. Helgason, 1984). In texture goniometry it was first noticed by Savelova (1982).

In complete analogy to (i) Fourier's harmonic method and (ii) d'Alembert's method of characteristics to solve an ordinary hyperbolic differential equation, e.g. to solve the Cauchy problem of mathematical physics (cf. Butzer and Nessel, 1971), the general solution of the ultrahyperbolic differential equation for hyperspherical X-ray transforms is obtained both in terms of (i) spherical harmonics and (ii) its characteristics.

The general solution of Eq. (6) in terms of harmonics is

$$P(\mathbf{h}, \mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{m'=-l}^{l} C_l^{mm'} (Y_l^m)^*(\mathbf{h}) Y_l^{m'}(\mathbf{r}) \qquad (7)$$

(Nikolayev and Schaeben, 1999).

Physical requirements like non-negativity, evenness, crystallographic or sample symmetries impose additional constraints on the system Eq. (7) and lead to special solutions.

The special case of considering $\mathbf{h}$ as constant leads to pole figures

$$P(\mathbf{h}, \mathbf{r}) = P_\mathrm{h}(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m'=-l}^{l} F_l^{m'}(\mathbf{h}) Y_l^{m'}(\mathbf{r}) \qquad (8)$$

with

$$F_l^{m'}(\mathbf{h}) = \sum_{m=-l}^{l} C_l^{mm'} (Y_l^m)^*(\mathbf{h}) \qquad (9)$$

The C-coefficients are calculated by inversion of Eq. (9), where the F-coefficients are provided by

$$F_l^{m'}(\mathbf{h}) = \int_{S^2} P(\mathbf{h}, \mathbf{r}) Y_l^{m'*}(\mathbf{r}) \, \mathrm{d}\, s(\mathbf{r}) \qquad (10)$$

if the right-hand side of Eq. (10) is accessible in some way.

The special case of considering $\mathbf{r}$ as constant leads to

analogous results with respect to inverse pole figures and their H-coefficients, respectively.

If accessible, F-coefficients are convenient, e.g. with respect to limited central memory for actual computations. In practical X-ray diffraction goniometry, they have never been accessible without additional provisions, because their numerical determination according to Eq. (10) requires completely measured pole figures. However, it is not possible to measure a complete pole figure in reflection nor in transmission mode of the texture goniometer. A complete experimental pole figure can be obtained by combining the intensity values of both modes, or by combining intensity values measured for three perpendicular surfaces of the specimen in one mode. In both cases, intensity data of different origin have to be fitted, which is apparently simple, but often leads to unacceptable results in practice.

Therefore, and since F-coefficients were believed to be an indispensable prerequisite of texture analysis from the projection point of view, Eqs. (1) and (2), they are numerically determined by a least-squares fit of a harmonic series of fixed maximum expansion degree $L_{\max}$ (cf. Bunge and Esling, 1985, p. 116). Unfortunately, when determined in this way, they depend on $L_{\max}$, thus losing their characteristic properties by definition Eq. (10) essential for orthogonal series expansion, and destroying the mathematical elegance of the harmonic approach.

Since the 'true' F-coefficients of experimental X-ray diffraction pole density functions are not accessible, the general solution, Eq. (7), applies, which relates C-coefficients directly to experimental intensities, e.g. if they are measured for many crystallographic but few sample directions.

Thus, F-coefficients have actually never been accessible in X-ray practice, but they are not generally required either. Therefore, they are obsolete from the complementary point of view provided by the differential Eq. (6).

The system of Eq. (7), may be augmented with

$$C_l^{mm'} = \frac{1}{\mathrm{vol}(B)} \sum_{k=1}^{N} \mathrm{vol}(B_k) D_l^{mm'}(g_k) \qquad (11)$$

where g_k denotes the individual orientation of the kth grain with volume $\mathrm{vol}(B_k)$, and $D_l^{mm'}$ denote the generalized spherical harmonics.

It is emphasized that Eq. (7) can be used to approximate additional pole figures directly from experimental intensity data. At the same time, the coefficients of the solution, Eq. (7), are the harmonic coefficients of the function being transformed (cf. Bunge, 1982, p. 53).

That is, any function satisfying a differential Eq. (6) can be shown to be the X-ray transform of a function under mild mathematical assumptions. More specifically, for any function $u \in C^{\infty}(S^2 \times S^2)$ satisfying the differential Eq. (6), there exists a unique function $f \in C^{\infty}(\mathrm{SO}(3))$ such that $\mathscr{P}_h f = u$ (Nikolayev and Schaeben, 1999).

It should be noted that if $u \in C^{\infty}(S^2 \times S^2)$ satisfying Eq. (6) is even in both arguments, then a unique even function $f \in C^{\infty}(\mathrm{SO}(3))$ exists such that $P_h f = u$. Since the crystallographic X-ray transforms of f are always even, uniqueness is confined to the even part of f under the crystallographic X-ray transform, i.e. only the even part of f is uniquely determined.

It follows that the statement that this common property of true pole figures $P_h(\mathbf{y})$ in no way follows from Eq. (6) or any transformed variants of it without additional information (Matthies and Esling, 1998, p. 214), is proven to be false, and so are its numerous paraphrases throughout their paper.

Thus, the coefficients of the solution, Eq. (7), of the differential equation for spherical X-ray transforms in terms of harmonics are the harmonic coefficients of the function being transformed, i.e. the solution of the differential equation provides the solution of the inverse X-ray transform problem. Whenever it is possible to determine the even part of an orientation density function conforming with given crystallographic pole figures of some crystal forms, then it is possible to determine directly the pole figure of any other crystal form, and vice versa. This possibility to solve a differential equation instead of an inverse transform problem has already been shown elsewhere. In particular, this duality may be exploited to improve on the conventionally obtained harmonic solution of the inverse problem of texture analysis.

Any function $u(\mathbf{h}, \mathbf{r}) \in C^2(S^2 \times S^2)$ which depends on the dot product $\mathbf{h} \cdot \mathbf{r} = \cos \eta$ only obviously satisfies the differential Eq. (6). Furthermore, an appropriate linear transformation of $\mathbf{h}$ or $\mathbf{r}$, respectively, with constant coefficients should not change this situation. Consequently, the characteristics of the ultrahyperbolic differential equation are the fibres $\mathbf{h} \cdot g\mathbf{r} = \mathrm{const.}$, where g is an arbitrary proper rotation of SO(3).

The general solution of Eq. (6) in terms of characteristics can be represented as

$$u(\mathbf{h}, \mathbf{r}) = \sum_l \sum_k u_l(\mathbf{h} \cdot g_k \mathbf{r}) \qquad (12)$$

where $g_k \in \mathrm{SO}(3)$ are arbitrary rotations and $u_l \in C^2(\mathrm{IR}^1)$ are some real twice differentiable functions (Nikolayev and Schaeben, 1999).

A specific solution is constructed analogously to d'Alembert's method of characteristics by choosing distinguished functions p_l for the functions u_l and fitting them to the initially given pole density figures, where the p_l belong to some specific dense subset of $C^2(\mathrm{IR}^1)$, e.g. polynomials, splines, wavelets or radial basis functions.

In a particularly simple case, a twice continuously differentiable function u satisfying Eq. (6) is considered, which reduces to a function of $\mathbf{h} \cdot g_0 \mathbf{r}$ for some arbitrary fixed $g_0 \in \mathrm{SO}(3)$. Then u is uniquely determined provided for some given $\mathbf{h}_0 \in S^2$ it is known for all $g_0 \mathbf{r}$ on a great circle containing h_0 (Nikolayev and Schaeben, 1999).

With respect to practical texture analysis these assumptions may appear rather artificial; nevertheless, this proposition is the basis of texture component fit methods (cf. Helming and Eschner, 1990; Schaeben, 1996). Moreover, the approach by characteristics can be greatly generalized to high resolution or multiresolution texture analysis.

It can generally be shown that a series expansion into appropriately chosen functions p_l is equivalent to the series expansion into spherical harmonics. Since any continuously differentiable function on the sphere S^2 can be expanded into an absolutely convergent series of spherical harmonics, there exists an equivalent expansion into linear combinations of specified spherical harmonics, the argument of which is the scalar product of $\mathbf{h}$ and $\mathbf{r}$ (cf. Freeden et al., 1998). This expansion provides the means to represent any pole density function in the form of Eq. (12).

For a more complete discussion on the subject including proofs the reader is referred to Nikolayev and Schaeben (1999).

3. Conclusions

It is shown that the approaches to texture analysis provided by the projection formula or the differential equation are equivalent, but put emphasis on different issues of the same problem. The possibility of applying a differential equation instead of an inverse tomographic problem has already been shown earlier, e.g. Bukhgeim (1988) and Patch (1998).

The latter approach provides a complementary and refreshing point of view and clearly reveals that the duality may be exploited to generalize and improve the conventional methods of texture analysis.

Eventually, it is shown that the basic statements by Matthies and Esling (1998) comprise an informal way to discuss the existence and uniqueness of the differential equation and that their arguments are essentially wrong— rather expressing personal opinions than mathematical facts. In particular, it is concluded that whenever it is possible to calculate a reasonable approximate of the even portion of an orientation density function conforming with experimental diffraction pole figures of given crystal forms, then it is possible to determine reasonable approximates of the pole figures of any other crystal form directly from the given ones, and vice versa.

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