WAVELET REPRESENTATION OF DIFFRACTION POLE FIGURES

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ABSTACT

Experimental diffraction pole figure data are thought of as being discretely sampled from pole density functions $P(\mathbf{h}, \mathbf{r})$, i.e. even probability density functions defined on the cross-product $S^2 \times S^2$ of two unit spheres. Several useful representations of pole density functions exist which are usually related to specific purposes: (i) series expansion into spherical harmonics, (ii) series expansion into (unimodal) radial basis functions, (iii) series expansion into piecewise constant functions. Their critical parameter may to some extent be adjusted to the total number and/or the spatial arrangement of the intensity measurements. However, they are in no way involved in the sampling process itself.
After briefly reviewing the basics of wavelets and the specifics of spherical wavelets, we introduce another representation of pole figures in terms of spherical wavelets. We will show that spherical wavelets are well suited to render pole figures, and to resolve the inverse problem. Moreover, we will demonstrate that wavelets are well apt to allow for locally varying spatial resolution, thus providing a digital device to zoom into pole figure areas of special interest. Considering a measuring time of roughly 1 hour for 1000 intensity values, such a device seems to be required to increase the spatial resolution by a factor of 1000 or greater locally. Eventually, we shall present a promising prospect that wavelets provide the means to control the texture goniometer and the sampling process to gradually adapt automatically to a local refinement of the spatial resolution.

REPRESENTATIONS OF POLE DENSITY FUNCTIONS

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

$$(\mathcal{P}_{\mathbf{h}} f)(\mathbf{r}) = \frac{1}{2\pi} \int_{\{g \in SO(3) \,|\, \mathbf{h} = g\mathbf{r}\}} f(g) dv(g) = P(\mathbf{h}, \mathbf{r}) \tag{1}$$

where the function $P(\mathbf{h}, \mathbf{r}) : S^2 \times S^2 \mapsto I\!R^1_+$ for a given crystallographic direction $\mathbf{h} \in S^2 \subset I\!R^3$ may be referred to as hyperspherical X–ray transform of f with respect to $\mathbf{h}$. The path of integration $\{g \in SO(3) | \mathbf{h} = g\mathbf{r}\}$ in (1) is a great–circle of the three-dimensional sphere $S^3 \subset I\!R^4$ parametrized by $\mathbf{h}$ and $\mathbf{r}$, cf. [8].
A crystallographic pole density function is the superposition of X-ray transforms with respect to crystal–symmetrically equivalent directions $\mathbf{h}_m, \;\; m = 1, \ldots, M_h$.
There are several representations of X-ray transforms and hence pole density functions, including the representation by

- series expansion into spherical harmonics

$$P(\mathbf{h},\mathbf{r}) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\sum_{m'=-\ell}^{\ell} C_\ell^{mm'}\overline{Y_\ell^m}(\mathbf{h})Y_\ell^{m'}(\mathbf{r}) \tag{2}$$
$$= \sum_{\ell=0}^{\infty}\sum_{m'=-\ell}^{\ell} F_\ell^{m'}(\mathbf{h})Y_\ell^{m'}(\mathbf{r})$$

  with

$$F_\ell^{m'}(\mathbf{h}) = \sum_{m=-\ell}^{\ell} C_\ell^{mm'}\overline{Y_\ell^m}(\mathbf{h})$$

  or

$$F_\ell^{m'}(\mathbf{h}) = \int_{S^2} P(\mathbf{h},\mathbf{r})\overline{Y_\ell^{m'}}(\mathbf{r})ds(\mathbf{r})$$

  respectively, to do mathematics,

- series expansion into (unimodal) radial basis functions

$$P(\mathbf{h},\mathbf{r}) = \sum_\ell w_\ell p(\mathbf{h}g_\ell\mathbf{r};\kappa(\ell)) \tag{3}$$

  e.g. with the de la Vallée Poussin kernel

$$p(\mathbf{h}g\mathbf{r};\kappa) = C(\kappa)\cos^{2\kappa}(\arccos(\mathbf{h}g\mathbf{r});\kappa)$$

  to do probability and statistics,

- series expansion into piecewise constant functions, i.e. indicators

$$P(\mathbf{h},\mathbf{r}) = \sum_{n=1}^{N}\frac{y_n(\mathbf{h})}{\mathrm{area}(Z_n)}\mathbb{1}_{Z_n}(\mathbf{r})$$

  with

$$y_n(\mathbf{h}) = \int_{Z_n} P(\mathbf{h},\mathbf{r})ds(\mathbf{r}),\ \ n = 1,\ldots,N$$

  for a partition of the upper (lower) hemisphere $S_+^2 \subset I\!R^3$ into surface patches $Z_n \subset S_+^2$, to do numerics.

It should be noted that the representations (2) and (3) are the general solutions in terms of harmonics or characteristics, resp., of the differential equation governing pole figures [8]. Thus, these representations prove useful in different ways to resolve the inverse problem of texture goniometry to reconstruct a reasonable orientation density function f defined on $SO(3)$, or equivalently on the hypersphere $S^3 \subset I\!R^4$, from the given intensity data which are mean values of f along great circles of S^3 parametrized by $\mathbf{h}$ and $\mathbf{r}$. Their critical parameter, e.g. (i) the degree of the harmonic series expansion, (ii) the window width (spherical dispersion) of the unimodal radial functions, (iii) the size of surface or volume elements where the functions are modelled to be constant, may to some extent be adjusted to the total number and/or the spatial arrangement of the intensity measurements. They are never involved in the sampling process itself.

A NEW REPRESENTATION WITH SPHERICAL WAVELETS

The main idea of wavelet analysis is to obtain a multiscale representation of the data or functions which allows localization in space and frequency. The advantages of such splittings have been used recently in a variety of applications (cf. [1]). In our case we start with the measured function values on a coarse almost equidistributed grid on the sphere S^2. These measurements are approximated by a spherical polynomial of low degree. This polynomial is clearly a sufficiently good approximation in regions of the sphere where the underlying function does not oscillate too much or in other words consists of low frequencies, only.
Now we need to improve this approximation in regions of the sphere where the original data set is very much oscillating. Therefore we need more measurements only locally. The crucial point is now the construction of a high degree polynomial from the global coarse grid and the local fine grid. This can be seen as adding adaptively and locally a wavelet part to the global approximation of low degree.
We define the inner product on the sphere with the surface element $d\mu$

$$\langle f, g \rangle = \frac{1}{4\pi} \int_{S^2} f(x)\overline{g}(x) d\mu(x)$$

and the norm $\|f\| = \langle f, f \rangle^{1/2}$. We say that $f : S^2 \to \mathbb{C}$ belongs to the Hilbert space $L^2(S^2)$ if $\|f\| < \infty$. By H_ℓ we denote the space of all spherical harmonics of degree ℓ with $\ell = 0, 1, 2, \ldots$; i.e. the restriction to the unit sphere of all homogeneous and harmonic polynomials in 3 variables. Then dim $H_\ell = 2\ell + 1$. The most important property of spherical harmonics for our approach are their orthogonality relations. Namely, for $p \in H_\ell$ and $q \in H_k$ with $\ell \neq k$ it holds $\langle p, q \rangle = 0$ and

$$L^2(S^2) = \overline{\bigoplus_{\ell=0}^{\infty} H_\ell}^{L^2} .$$

Further we denote $\Pi_n = \bigoplus_{\ell=0}^{n} H_\ell$ with $\dim \Pi_n = (n+1)^2$. This orthogonal decomposition gives rise to look for bases localized in space and frequency domain.
To formalize the notation let in the following $\{N_j\}$ be a sequence of strictly monotone increasing positive integers.
Then we introduce the so-called scaling space V_j as a polynomial space

$$V_j = \Pi_{N_j}$$

with dim $V_j = (N_j + 1)^2$. Hence we have a chain

$$V_0 \subset V_1 \subset V_2 \subset \ldots$$

and it makes sense to define the corresponding orthogonal complements

$$W_j = V_{j+1} \ominus V_j = \bigoplus_{\ell=N_j+1}^{N_{j+1}} H_\ell$$

with $\dim W_j = (N_{j+1} - N_j)(N_{j+1} + N_j + 2)$. Finally we obtain

$$L^2(S^2) = \overline{V_0 \oplus \bigoplus_{j=0}^{\infty} W_j}^{L^2} .$$

The classical approach of wavelet theory uses $N_j = 2^j$. But in case of the surface this would imply a very large dimension of the wavelet spaces. Therefore our choice in the calculations is more like $N_j = 20j$.

Up to now we can think of a frequency-localized decomposition of $L^2(S^2)$. Now the main question is to obtain bases for the different spaces W_j which are also localized in space. The basic idea to achieve this goal is based on the addition formula. Namely, for every orthonormal basis $\{Y_{\ell,k}, k = -\ell, \ldots, \ell\}$ of H_ℓ it holds

$$\sum_{k=-\ell}^{\ell} Y_{\ell,k}(x)\overline{Y_{\ell,k}}(y) = \frac{2\ell+1}{4\pi} P_\ell(x \cdot y), \qquad x, y \in S^2,$$

where P_ℓ is the Legendre polynomial of degree ℓ with $P_\ell(1) = 1$. In particular, for suitably chosen points $\xi_k, k = -\ell, \ldots, \ell$ the functions $P_\ell(\xi_k \cdot \circ)$ yield a basis for H_ℓ. Analogously, there exist $(N_j+1)^2$ points $\eta_k, k = 1, \ldots, (N_j+1)^2$ on the unit sphere so that

$$\sum_{\ell=0}^{N_j} (2\ell+1) P_\ell(\eta_k \cdot \circ)$$

is a basis for V_j. Unfortunately, it is very difficult on the one hand to find such η_k and on the other hand to compute these sums efficiently. Hence, it is more suitable to take an oversampling approach as in [6, 7]. Therefore we parametrize the points $x \in S^2$ by their spherical coordinates $(\theta, \phi) \in [0, \pi] \times [0, 2\pi)$.

Let us assume in the sequel that we can compute functions at the grid I_j consisting of points

$$\xi_{s,t}^j = \left(\frac{\pi s}{2N_j}, \frac{\pi t}{N_j} \right), \qquad s = 0, \ldots, 2N_j, \quad t = 0, \ldots, 2N_j - 1.$$

Using the Clenshaw-Curtis quadrature formula and the trapezoidal rule it holds for every $Q, R \in V_j$

$$\frac{1}{4\pi} \int_{S^2} Q(x) R(x) d\mu(x) = {\sum_{s=0}^{2N_j}}' \sum_{t=0}^{2N_j-1} w_s^j \, Q(\xi_{s,t}^j) R(\xi_{s,t}^j) \tag{4}$$

with the Clenshaw-Curtis weights

$$w_s^j = \frac{-1}{N_j} {\sum_{u=0}^{N_j}}' \frac{1}{4u^2 - 1} \cos \frac{su\pi}{N_j}.$$

Here $\sum'$ means that the first and last term in the sum will be multiplied by $1/2$.

With (4) we are able to compute in an approximate way the orthogonal projection S_V into V_j as

$$\begin{aligned} S_V f(x) &= \sum_{\ell=0}^{N_j} \sum_{k=1}^{2\ell+1} \langle f, Y_{\ell,k} \rangle Y_{\ell,k}(x) \\ &= \sum_{\ell=0}^{N_j} \langle f, \frac{2\ell+1}{4\pi} P_\ell(x \cdot \circ) \rangle. \end{aligned}$$

Analogously, we write the orthogonal projection S_W into W_j as

$$S_W f(x) = \sum_{\ell=N_j+1}^{N_{j+1}} \langle f, (2\ell+1) P_\ell(x \cdot \circ) \rangle.$$

Introducing the kernels

$$G_j(t) = \sum_{\ell=0}^{N_j} (2\ell+1) P_\ell(t)$$

and

$$H_j(t) = \sum_{\ell=N_j+1}^{N_{j+1}} (2\ell+1) P_\ell(t)$$

we compute the approximations as

$$S_V^I f(x) = {\sum_{s=0}^{2N_j}}' \sum_{t=0}^{2N_j-1} w_s^j \; f(\xi_{s,t}^j) \; G_j(\xi_{s,t}^j \cdot x)$$

and

$$S_W^I f(x) = {\sum_{s=0}^{2N_{j+1}}}' \sum_{t=0}^{2N_{j+1}-1} w_s^{j+1} \; f(\xi_{s,t}^{j+1}) \; H_j(\xi_{s,t}^{j+1} \cdot x).$$

Now the proposed procedure is the following. We know the function on a coarse grid and compute $S_V^I f(x)$. By inspection we find the parts of the surface where f and $S_V^I f$ have large absolute values and large oscillations, respectively.
Let us note here that there exist also algorithms to detect these areas based on multiresolution. We do not go into the details here (cf. [4]).
In the next step we want to improve our approximation $S_V^I f$ by adding the next wavelet part $S_W^I f$. Unfortunately, we are not able to calculate f on a whole fine grid but we know that $S_W^I f$ is almost zero in regions where f does noch oscillate too much.
Therefore we replace $S_V^I f + S_W^I f$ by $S_V^I f + \tilde{S}_W^I f$ where

$$\tilde{S}_W^I f = {\sum_{s=0}^{2N_{j+1}}}' \sum_{t=0}^{2N_{j+1}-1} w_s^{j+1} \; L_j f(\xi_{s,t}^{j+1}) \; H_j(\xi_{s,t}^{j+1} \cdot \circ)$$

and

$$L_j f(\xi_{s,t}^{j+1}) = \begin{cases} f(\xi_{s,t}^{j+1}) & \text{if } f \text{ is large,} \\ S_V^I f(\xi_{s,t}^{j+1}) & \text{otherwise.} \end{cases}$$

The definition of L_j shows that we have to compute the function values only on the coarse grid and on some additional values where we expect big oscillations of f.

EXAMPLE

The example was designed with standard functions [2] and resembles features of the SANTA FE cubic-orthorhombic data [3], which were composed of a single Fisher component weighted 0.27 with center $g_0 = (63.435, 48.190, 63.435)$ and halfwidth of 20 degrees and a uniform portion of 0.73 (see Table 1). Our DENVER cubic-orthorhombic data set is composed of a first Fisher component weighted 0.235 with center $g_0 = (63.435, 50.190, 63.435)$ and halfwidth of 20 degrees, a second Fisher component weighted 0.035 with the same center and a halfwidth of 1 degree, and a uniform portion of 0.73 (see Table 1).

Table 1: Range of pole figures vs. grid refinement

Reflection Range	(100) min	 max	(110) min	 max	(111) min	 max	(311) min	 max
SANTA FE 5×5	0.730	4.786	0.730	2.723	0.730	3.723	0.736	1.746
DENVER 5×5	0.730	4.253	0.730	3.679	0.730	4.201	0.735	36.503
DENVER 2.5×2.5	0.730	63.103	0.730	57.577	0.730	40.097	0.735	45.956
DENVER 1×1	0.730	208.999	0.730	80.821	0.730	147.893	0.734	53.821
DENVER 0.5×0.5	0.730	202.281	0.730	107.138	0.730	160.485	0.734	54.048
DENVER 0.1×0.1	0.730	215.028	0.730	108.223	0.730	161.797	0.734	54.534

Table 2: l_2 and l_∞ error of (100) pole figure of DENVER 1×1 vs. polynomial degree

	100% of data used		25.3% of data used		6.6% of data used	
polynomial degree	l_∞	l_2	l_∞	l_2	l_∞	l_2
50	1890	4198	1899	4202	1899	4198
100	1506	3455	1505	3449	1505	3452
150	950	2456	960	2459	960	2456
200	372	1504	372	1498	372	1504

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