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# High Resolution Texture Analysis with Spherical Wavelets

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**Abstract.** The representations of both orientation and pole density functions in terms of spherical wavelets are exposed and their properties and relationship are discussed. The main idea of wavelet analysis is to obtain a multiscale representation of the functions or the data which allows localization in space and frequency. This mainstream idea of modern data analysis is adapted to texture analysis.

Initially the pole figures are scanned on a coarse grid and a first rough approximation of the orientation density function by low-order wavelets is calculated. Next, areas of specific interest in orientation space, e.g. large values, large gradients, etc. of the first approximation, are interactively defined or automatically detected, and the assumption is imposed that the first approximation is sufficiently good everywhere else. Next, the pole figures patches corresponding to the distinguished area of orientation space are determined employing the geometry of the orientation-to-pole projection. Then the initial coarse grid is refined and additional intensities are sampled for the refined grid locations within the distinguished surface patches. Outside the surface patches, intensities associated to the grid locations are numerically determind form the first approximation of the orientation density function. Based on the additional experimental intensity data and the calculated intensities a new wavelet approximation of larger order is calculated. It improves the approximation of the orientation density function in the areas of specific interest and leaves the first rough approximation almost unchanged elsewhere. Thus, it approximates the experimental data according to both the coarse and the refined grid. This procedure may be iterated until the improvement can be neglected. The method seems appropriate to evaluate synchrotron radiation data and to resolve the "orientation distribution within a single crystal".

Also, the approach by spherical wavelets provides a means to control the sampling process of pole density functions to gradually adapt automatically to a local refinement of the spatial resolution.

## Introduction

The orientation of an individual crystal is given by the rotation $\boldsymbol{g} \in SO(3)$ which brings a right–handed orthogonal coordinate system $K_S$ fixed to the specimen into coincidence with

another right–handed orthogonal coordinate system $K_C$ fixed to the crystal, $\boldsymbol{g} : K_S \mapsto K_C$. Then the coordinates of a unique direction represented by $\mathbf{h} \in S^2 \subset \mathbb{R}^3$ with respect to the crystal coordinate system $K_C$ (referred to a crystallographic direction) and by $\mathbf{r} \in S^2$ with respect to the specimen coordinate system $K_S$ (referred to as specimen direction) are related to each other by $\mathbf{r} = \boldsymbol{g}\mathbf{h}$.

Texture analysis with X–ray or neutron diffraction data is the analysis of the orientation distribution by volume in terms of an orientation probability density function $f : SO(3) \mapsto \mathbb{R}_+$ and its corresponding experimentally accessible pole probability density functions $(Pf)_h(\mathbf{r}) : S^2 \mapsto \mathbb{R}_+$ which represent the probability that a (fixed) crystal direction $\mathbf{h}$ or its antiparallel $-\mathbf{h}$ statistically coincides with the specimen direction $\mathbf{r}$. With respect to the experiment the feasible crystal directions are the normals of the crystallographic lattice planes. An even crystallographic pole probability density function

$$(\mathcal{X}f)(\mathbf{h},\mathbf{r}) := \sum_{\mathbf{h}\in\hbar} \frac{1}{2}\Big((\mathcal{R}f)(\mathbf{h},\mathbf{r}) + (\mathcal{R}f)(-\mathbf{h},\mathbf{r})\Big) = P(\mathbf{h},\mathbf{r}) \tag{1}$$

of the crystal form $\hbar$, where $\hbar$ denotes the set of all symmetrically equivalent crystallographic directions $\mathbf{h}$, is basically provided by superpositions of the spherical Radon transform of the orientation probability density function $f : SO(3) \mapsto \mathbb{R}$ defined as

$$(\mathcal{R}f)(\mathbf{h},\mathbf{r}) := \frac{1}{2\pi} \int_{G(\mathbf{h},\mathbf{r})} f(\boldsymbol{g})\, d\boldsymbol{g} \tag{2}$$

with the path of integration $G(\mathbf{h},\mathbf{r}) = \{\boldsymbol{g} \in SO(3) \,|\, \mathbf{r} = \boldsymbol{g}\mathbf{h}\}$, cf. [1], [6].

Like general Radon, $k$–plane or X–ray transforms (cf. Helgason [4], [5]) the spherical Radon transform of a function and hence crystallographic pole probability density functions ("pole figures") satisfy a Darboux–type differential equation

$$(\Delta_{\mathbf{h}} - \Delta_{\mathbf{r}})(\mathcal{R}f)(\mathbf{h},\mathbf{r}) = 0 \tag{3}$$

(Savyolova [9]) with the Laplace–Beltrami operator $\Delta$. Its general solution in terms of spherical harmonics $Y_\ell^m$ is

$$A(\mathbf{h},\mathbf{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} C_\ell^{mn}\, \overline{Y_\ell^m}(\mathbf{h})\, Y_\ell^n(\mathbf{r}) \tag{4}$$

and the function $A : S^2 \times S^2 \mapsto \mathbb{R}$ is the spherical Radon transform of

$$f(\boldsymbol{g}) = \frac{1}{\sqrt{4\pi}} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} \frac{1}{\sqrt{2\ell+1}}\, C_\ell^{mn}\, T_\ell^{mn}(\boldsymbol{g}) \tag{5}$$

(Nikolayev and Schaeben [8]) with generalized spherical harmonics $T_\ell^{mn}$. Thus, solving the differential equation (3) is equivalent to inverting the spherical Radon transform.

The fibre, i.e. the path of integration $G(\mathbf{h},\mathbf{r}) = \{\boldsymbol{g} \in SO(3) \,|\, \mathbf{r} = \boldsymbol{g}\mathbf{h}\}$ in equation (1), may be represented by the circle of rotations $C$ spanned by any two different rotations $\boldsymbol{g}_1, \boldsymbol{g}_2$ mapping $\mathbf{h}$ onto $\mathbf{r}$. The circle itself may be parametrized by

$$C(\boldsymbol{g}_1(\mathbf{h},\mathbf{r}), \boldsymbol{g}_2(\mathbf{h},\mathbf{r})) = \{\boldsymbol{g}(\omega;\mathbf{r})\, \boldsymbol{g}_0 \,|\, \omega \in [0, 2\pi)\},$$

where $\boldsymbol{g}_0$ denotes an arbitrarily fixed element of the fibre, and $\boldsymbol{g}(\omega;\mathbf{r})$ denotes a rotation about $\mathbf{r}$ by $\omega \in [0, 2\pi)$. Then, the defining equation (1) of the spherical Radon transform of $f$ may be explicitly rewritten as

$$(\mathcal{R}f)(\mathbf{h},\mathbf{r}) = \frac{1}{2\pi}\int_0^{2\pi} f(\boldsymbol{g}(\omega;\mathbf{r})\,\boldsymbol{g}_0)\,d\omega. \tag{6}$$

The invariant Haar measure in eq.(6) is $d\omega$ which follows from the postulate that the measurements should essentially be independent of the choices of the involved coordinate systems $K_S, K_C$, which in turn requires that the relation of an orientation probability density function and its Radon transform satisfy an invariance of the form

$$\mathcal{R}[f(\circ)](\mathbf{h},\mathbf{r}) = \mathcal{R}[f(\boldsymbol{g}_1^{-1}\circ\boldsymbol{g}_2)](\boldsymbol{g}_2\mathbf{h},\boldsymbol{g}_1\mathbf{r})$$

for arbitrary $\boldsymbol{g}_1, \boldsymbol{g}_2 \in SO(3)$.

Without refering to any specific crystal or specimen symmetry crystallographic pole probability density functions are superpositions of the spherical Radon transforms with respect to the two physically indistinguishable lattice plane normals $\mathbf{h}$ and $-\mathbf{h}$. Thus, regardless of the actual crystal or specimen symmetry, the effective symmetry is always the corresponding Laue–class symmetry.

In case of symmetries, crystallographic pole probability density functions are again superpositions of the spherical Radon transforms with respect to the symmetrically equivalent and physically indistinguishable lattice planes normals and their antipodally symmetric directions.

If $f$ satisfies any symmetry relation

$$f(\boldsymbol{g}_s^{-1}\boldsymbol{g}\boldsymbol{g}_c) = f(\boldsymbol{g}),$$

then

$$(\mathcal{R}f)(\boldsymbol{g}_c\mathbf{h},\boldsymbol{g}_s\mathbf{r}) = (\mathcal{R}f)(\mathbf{h},\mathbf{r}),$$

and the harmonic representations may be rewritten in terms of symmetrized harmonics

$$f(\boldsymbol{g}) = \sum_{\ell=0}^{\infty}\sum_{\mu=1}^{M(\ell)}\sum_{\nu=1}^{N(\ell)} C_\ell^{\mu\nu}\,\ddot{T}_\ell^{\mu\nu}(\boldsymbol{g}),\quad (\mathcal{R}f)(\mathbf{h},\mathbf{r}) = \sum_{\ell=0}^{\infty}\sum_{\mu=1}^{M(\ell)}\sum_{\nu=1}^{N(\ell)} C_\ell^{\mu\nu}\,\overline{\dot{Y}_\ell^{\mu}}(\mathbf{h})\,\dot{Y}_\ell^{\nu}(\mathbf{r})$$

with symmetrized harmonics $\ddot{T}_\ell^{\mu\nu}(\boldsymbol{g})$ and $\dot{Y}_\ell^{\mu}(\mathbf{h})$, $\dot{Y}_\ell^{\nu}(\mathbf{r})$, respectively, which are certain linear combinations of the common harmonics, e.g.

$$\ddot{T}_\ell^{\mu\nu}(\boldsymbol{g}) = \sum_{m=-\ell}^{\ell}\sum_{n=-\ell}^{\ell} \dot{a}_\ell^{m\mu}\,\dot{a}_\ell^{n\nu}\,T_\ell^{mn}(\boldsymbol{g}).$$

The spherical Radon transform has the property

$$(\mathcal{R}T_\ell^{mn})(\mathbf{h},\mathbf{r}) = \frac{1}{\sqrt{4\pi}}\frac{1}{\sqrt{2\ell+1}}\,\overline{Y_\ell^m}(\mathbf{h})\,Y_\ell^n(\mathbf{r}), \tag{7}$$

which provides a singular value decomposition with respect to the spaces $\mathcal{L}^2(SO(3))$ and $\mathcal{L}^2(\mathbb{S}^2\times\mathbb{S}^2)$, respectively.

Thus, the spherical Radon transform maps any linear combination of generalized spherical harmonics onto the linear combination of spherical harmonics with the same harmonic coefficients. Since

$$(\mathcal{X}T_\ell^{mn})(\mathbf{h},\mathbf{r}) = \begin{cases} \frac{1}{\sqrt{4\pi}}\frac{1}{\sqrt{2\ell+1}}\overline{Y_\ell^m}(\mathbf{h})\,Y_\ell^n(\mathbf{r}), & \text{if } \ell \text{ even} \\ 0, & \text{if } \ell \text{ odd} \end{cases} \tag{8}$$

only the "even" part of an orientation probability density function can approximately be retrieved from experimental intensities $\iota(\hbar_i,\mathbf{r}_i) \approx P(\mathbf{h}_i,\mathbf{r}_i)$ without additional modeling assumptions. The canonical modeling assumption provided by the non–negativity constraint $f \geq 0$ may be realized by a maximum entropy approach.

### Spherical wavelet representation of the spherical Radon transform

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. Freeden et al [3]). Initially, the experimentally accessible $\hbar$–pole probability density function $(Pf)_\hbar(\circ) = P(\mathbf{h},\circ)$ is sampled 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. This approximation requires improvement in regions of the sphere where the initial data are largely oscillating. Therefore, additional measurements are required only locally. The crucial point is now the construction of a high degree polynomial from the globally coarse grid and the locally refined grid. This can be seen as adding adaptively and locally a wavelet part to the global approximation of low degree.

Keeping in mind that with respect to the diffraction experiment the direction $\mathbf{h}$ is rather a parameter than a variable of $\mathcal{R}f$ and $P(\mathbf{h},\circ)$, respectively, which may therefore be considered as functions $(Pf)_\hbar : \mathbb{S}^2 \mapsto \mathbb{R}_+$, the major steps of the wavelet representation of $\mathcal{R}f$ in the variable $\mathbf{r}$ will be presented next.

Reordering the sum (4) yields

$$\begin{aligned}(\mathcal{R}f)(\mathbf{h},\mathbf{r}) &= \sum_{\ell=0}^{\infty}\sum_{n=-\ell}^{\ell}\left[\sum_{m=-\ell}^{\ell} C_\ell^{mn}\overline{Y_\ell^m}(\mathbf{h})\right]Y_\ell^n(\mathbf{r}) = \sum_{\ell=0}^{\infty}\sum_{n=-\ell}^{\ell} F_n^\ell(\mathbf{h})\,Y_\ell^n(\mathbf{r}) \\ &= \sum_{\ell=0}^{\infty}\sum_{n=-\ell}^{\ell}\Big\langle(\mathcal{R}f)(\mathbf{h},\circ),Y_\ell^n(\circ)\Big\rangle Y_\ell^n(\mathbf{r}) \end{aligned} \tag{9}$$

with the inner product on the sphere with the surface element $ds$

$$\langle A,B\rangle = \int_{S^2} A(\mathbf{r})\,\overline{B(\mathbf{r})}ds(\mathbf{r}).$$

The space of all spherical harmonics of degree $\ell$ with $\ell = 0,1,2,\ldots$, i.e. the restriction to the unit sphere $\mathbb{S}^2$ of all homogeneous and harmonic polynomials in 3 variables, is denoted by $\mathcal{Y}_\ell$; then $\dim \mathcal{Y}_\ell = 2\ell+1$. The most important property of spherical harmonics here is their orthogonality relation. Namely, for $Y_\ell^m \in \mathcal{Y}_\ell$ and $Y_k^n \in \mathcal{Y}_k$ with $\ell \neq k$ it is $\langle Y_\ell^m, Y_k^n\rangle = 0$ and

$$\mathcal{L}^2(S^2) = \overline{\bigoplus_{\ell=0}^{\infty}\mathcal{Y}_\ell}^{\mathcal{L}^2},$$

i.e. any function in $\mathcal{L}^2(S^2)$ may be represented by its harmonic series expansion. Further, $\Pi_n(S^2) = \bigoplus_{\ell=0}^{n} \mathcal{Y}_\ell$ with $\dim \Pi_n(S^2) = (n+1)^2$. Next we introduce increasing "packages" of finite harmonic spaces in such a way that the actual package contains the preceeding one, and we shall refer to them as scaling spaces. Organized in this way, the harmonic spaces will give rise to a multi–scale representation.

Let $\{N_j\}$ be a sequence of strictly monotone increasing positive integers. Then scaling spaces $V_j$ are introduced as polynomial spaces

$$V_j(S^2) = \Pi_{N_j}(S^2)$$

with $\dim V_j(S^2) = (N_j+1)^2$. Hence there is a chain

$$V_0(S^2) \subset V_1(S^2) \subset V_2(S^2) \subset \ldots$$

and it is sensible to define the corresponding orthogonal complements

$$W_j(S^2) = V_{j+1}(S^2) \ominus V_j(S^2) = \bigoplus_{\ell=N_j+1}^{N_{j+1}} \mathcal{Y}_\ell$$

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

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

The classical approach of wavelet theory uses $N_j = 2^j$. However, in case of pole probability density functions defined on the unit sphere this would imply very large dimensions of the wavelet spaces. Therefore our choice in the calculations is more like $N_j = 20j$.

Using now

$$\sum_{k=-\ell}^{\ell} Y_\ell^k(\mathbf{r}_1)\,\overline{Y_\ell^k}(\mathbf{r}_2) = \frac{2\ell+1}{4\pi} P_\ell(\mathbf{r}_1 \cdot \mathbf{r}_2), \quad \mathbf{r}_1, \mathbf{r}_2 \in S^2$$

with Legendre polynomials $P_\ell$ of degree $\ell$ with $P_\ell(1) = 1$ results in

$$(\mathcal{R}f)(\mathbf{h}, \mathbf{r}) = \sum_{\ell=0}^{\infty} \left\langle (\mathcal{R}f)(\mathbf{h}, \circ), \frac{2\ell+1}{4\pi} P_\ell(\mathbf{r} \cdot \circ) \right\rangle . \tag{10}$$

Considering harmonics only up to order $N_j$ the approximation $S_{V_j}(\mathcal{R}f)(\mathbf{h}, \mathbf{r})$ with respect to $V_j$ is given by

$$S_{V_j}(\mathcal{R}f)(\mathbf{h}, \mathbf{r}) = \sum_{\ell=0}^{N_j} \left\langle (\mathcal{R}f)(\mathbf{h}, \circ), \frac{2\ell+1}{4\pi} P_\ell(\mathbf{r} \cdot \circ) \right\rangle \tag{11}$$

and the corresponding next wavelet part by

$$S_{W_j}(\mathcal{R}f)(\mathbf{h}, \mathbf{r}) = \sum_{N_j+1}^{N_{j+1}} \left\langle (\mathcal{R}f)(\mathbf{h}, \circ), \frac{2\ell+1}{4\pi} P_\ell(\mathbf{r} \cdot \circ) \right\rangle . \tag{12}$$

Introducing the kernel

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

yields

$$S_{V_j}(\mathcal{R}f)(\mathbf{h},\mathbf{r}) = \frac{1}{4\pi} \int_{S^2} (\mathcal{R}f)(\mathbf{h},\mathbf{r}')\, \widetilde{G}_j(\mathbf{r}\cdot\mathbf{r}')\, ds(\mathbf{r}') \tag{13}$$

where the right hand side is spatially localized and can be numerically evaluated by

$$S^I_{V_j}(\mathcal{R}f)(\mathbf{h},\mathbf{r}) = \sum_{k=1}^{K_j} w'_j(k)\, (\mathcal{R}f)(\mathbf{h},\mathbf{r}'_{j,k})\, \widetilde{G}_j(\mathbf{r}\cdot\mathbf{r}'_{j,k}) \tag{14}$$

applying the Clenshaw–Curtis quadrature formula and the trapezoidal rule with appropriately chosen $\mathbf{r}_{j,k} \in S^2, k = 1,\ldots,K_j$.

Analogously, setting

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

yields

$$S^I_{W_j}(\mathcal{R}f)(\mathbf{h},\mathbf{r}) = \sum_{k=1}^{K_{j+1}} w'_{j+1}(k)\, (\mathcal{R}f)(\mathbf{h},\mathbf{r}'_{j+1,k})\, \widetilde{H}_j(\mathbf{r}\cdot\mathbf{r}'_{j+1,k}) \tag{15}$$

and results in

$$S^I_{V_{j+1}}(\mathcal{R}f)(\mathbf{h},\mathbf{r}) = S^I_{V_j}(\mathcal{R}f)(\mathbf{h},\mathbf{r}) + S^I_{W_j}(\mathcal{R}f)(\mathbf{h},\mathbf{r}). \tag{16}$$

Substituting $S^I_{W_j}(\mathcal{R}f)(\mathbf{h},\mathbf{r})$ by

$$\hat{S}^I_{W_j}(\mathcal{R}f)(\mathbf{h},\mathbf{r}) = \sum_{k=1}^{K_{j+1}} w'_{j+1}(k)\, L_j(\mathcal{R}f)(\mathbf{h},\mathbf{r}'_{j+1,k})\, H_j(\mathbf{r}\cdot\mathbf{r}'_{j+1,k}) \tag{17}$$

with

$$L_j(\mathcal{R}f)(\mathbf{h},\mathbf{r}_{j+1,k}) = \begin{cases} (\mathcal{R}f)(\mathbf{h},\mathbf{r}_{j+1,k}) & \text{if } (\mathcal{R}f) \text{ is large,} \\ S^I_V(\mathcal{R}f)(\mathbf{h},\mathbf{r}_{j+1,k}) & \text{otherwise,} \end{cases} \tag{18}$$

eventually yields

$$\hat{S}^I_{V_{j+1}}(\mathcal{R}f)(\mathbf{h},\mathbf{r}) = S^I_{V_j}(\mathcal{R}f)(\mathbf{h},\mathbf{r}) + \hat{S}^I_{W_j}(\mathcal{R}f)(\mathbf{h},\mathbf{r}). \tag{19}$$

The wavelet representation of $(\mathcal{R}f)(\mathbf{h},\mathbf{r})$ in the variable $\mathbf{r}$ can immediately be applied to $(\mathcal{X}f)(\mathbf{h},\mathbf{r})$ read as a function $(Pf)_\hbar(\mathbf{r})$.

Summarizing, the proposed procedure is as follows. The function $(Pf)_\hbar(\mathbf{r})$ is known on a coarse $\mathbf{r}$–grid and $S^I_V(Pf)_\hbar(\mathbf{r})$ is computed. By inspection or algorithms (cf. Mhaskar et al. [7]) the regions of the pole figure where $(Pf)_\hbar(\mathbf{r})$ and $S^I_V(Pf)_\hbar(\mathbf{r})$ have large absolute values and large oscillations, respectively, are detected. In the next step the approximation $S^I_V(Pf)_\hbar$ is improved by adding the next wavelet part $S^I_W(Pf)_\hbar$. Since $(Pf)_\hbar(\mathbf{r})$ cannot be totally sampled on a refined $\mathbf{r}$–grid and since it is known that $S^I_W(Pf)_\hbar$ is almost zero in regions where $(Pf)_\hbar(\mathbf{r})$ does noch oscillate too much, $S^I_V(Pf)_\hbar + S^I_W(Pf)_\hbar$ is replaced by $S^I_V(Pf)_\hbar) + \hat{S}^I_W(Pf)_\hbar$. The definition of $L_j$ shows that the pole figure $(Pf)_\hbar(\mathbf{r})$ must be resampled for some additional points in the regions where large oscillations of $(Pf)_\hbar(\mathbf{r})$ are observed or expected.

**Generalized spherical wavelet representation of orientation probability density functions**

We shall pursue an analogous approach towards a spherical wavelet representation of the orientation probability density function as above. In particular, we shall construct a chain of scaling spaces and see that the Radon transform of the corresponding wavelet representation can be identified with the wavelet representation of the Radon transform developed above.

The space of generalized (hyperspherical) harmonic functions $T_\ell^{mn}, m,n = -\ell,\ldots,\ell$, is denoted by $\mathcal{T}_\ell, \ell = 0,1,\ldots$; then $\dim \mathcal{T}_\ell = (2\ell+1)^2$. It is

$$\left\langle T_\ell^{mn}, T_{\ell'}^{m'n'} \right\rangle = 0, \quad \ell \neq \ell',$$

and

$$\mathcal{L}^2(SO(3)) = \overline{\bigoplus_{\ell=0}^{\infty} \mathcal{T}_\ell}^{\mathcal{L}^2},$$

i.e. any function in $\mathcal{L}^2(SO(3))$ may be represented by its generalized harmonic series expansion

$$f(\boldsymbol{g}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} C_\ell^{mn} T_\ell^{mn}(\boldsymbol{g}).$$

The space of generalized harmonics of degree at most $n$ is denoted by $\Pi_n(SO(3)) = \bigoplus_{\ell=0}^{n} \mathcal{T}_\ell$ with $\dim \Pi_n(SO(3)) = (n+1)\big(4(n+1)^2-1\big)/3$. Let $N_j$ be a sequence of strictly monotone increasing positive integers. The space

$$V_j(SO(3)) = \Pi_{N_j}(SO(3))$$

with $\dim V_j(SO(3)) = (N_j+1)\big(4(N_j+1)^2-1\big)/3$ is referred to as scaling space and its definition gives rise to a chain of scaling spaces

$$V_0(SO(3)) \subset V_1(SO(3)) \subset V_2(SO(3)) \subset \ldots .$$

Its corresponding orthogonal complements are defined by

$$W_j(SO(3)) = V_{j+1}(SO(3)) \ominus V_j(SO(3)) = \bigoplus_{\ell=N_j+1}^{N_{j+1}} \mathcal{T}_\ell$$

with $\dim W_j(SO(3)) = \dim V_{j+1}(SO(3)) - \dim V_j(SO(3))$. Eventually, it is

$$\mathcal{L}^2(SO(3))) = \overline{V_0(SO(3)) \oplus \bigoplus_{j=0}^{\infty} W_j(SO(3))}^{\mathcal{L}^2}.$$

The generalized harmonics satisfy

$$\sum_{m,n=-\ell}^{\ell} T_\ell^{mn}(\boldsymbol{g}_1)\overline{T_\ell^{mn}}(\boldsymbol{g}_2) = (2\ell+1)U_{2\ell}\Big(\frac{\omega(\boldsymbol{g}_1,\boldsymbol{g}_2)}{2}\Big) = (2\ell+1)^2 C_\ell^{(1)}\Big(\frac{\omega(\boldsymbol{g}_1,\boldsymbol{g}_2)}{2}\Big), \quad \boldsymbol{g}_1,\boldsymbol{g}_2 \in SO(3)$$

with the even–order Chebyshev polynomials of second kind $U_{2\ell}(x/2) = \frac{\sin(2\ell+1)x/2}{\sin x/2}$) (synonymously Dirichlet kernel), or Gegenbauer polynomials $C_\ell^{(1)}$ of order $\ell$ with $C_\ell^{(1)}(1) = 1$.

The orthogonal projection $S_V f$ of $f$ into $V_j(SO(3))$ is defined as

$$S_{V_j} f(\boldsymbol{g}) := \sum_{\ell=0}^{N_j} \sum_{m=-\ell}^{\ell} \sum_{n=-\ell}^{\ell} \left\langle f(\circ), T_\ell^{mn}(\circ) \right\rangle T_\ell^{mn}(\boldsymbol{g}) = \sum_{\ell=0}^{N_j} \left\langle f(\circ), (2\ell+1)^2 C_\ell^{(1)}(\frac{\omega(\boldsymbol{g}, \circ)}{2}) \right\rangle, \quad (20)$$

and analogously

$$S_{W_j} f(\boldsymbol{g}) := \sum_{\ell=N_j+1}^{N_{j+1}} \left\langle f(\circ), (2\ell+1)^2 C_\ell^{(1)}(\frac{\omega(\boldsymbol{g}, \circ)}{2}) \right\rangle \quad (21)$$

such that

$$S_{V_{j+1}} f(\boldsymbol{g}) = S_{V_j} f(\boldsymbol{g}) + S_{W_j} f(\boldsymbol{g}). \quad (22)$$

Introducing the kernels

$$G_j(t) = \sum_{\ell=0}^{N_j} (2\ell+1)^2 C_\ell^{(1)}(t/2), \text{ and } H_j(t) = \sum_{\ell=N_j+1}^{N_{j+1}} (2\ell+1)^2 C_\ell^{(1)}(t/2)$$

yields

$$S_{V_j} f(\boldsymbol{g}) = \int_{SO(3)} f(\boldsymbol{g}') \, G_j(\cos \frac{\omega(\boldsymbol{g}', \boldsymbol{g})}{2}) \, d\boldsymbol{g}' \quad (23)$$

which can be numerically evaluated by

$$S_{V_j}^I f(\boldsymbol{g}) = \sum_{k=1}^{K_j} w_j(k) \, f(\boldsymbol{g}_{j,k}) \, G_j(\cos \frac{\omega(\boldsymbol{g}_{j,k}, \boldsymbol{g})}{2}). \quad (24)$$

Applying the sphercial Radon transform we get

$$\begin{aligned} (\mathcal{R}[(S_{V_j}^I f(\circ))])(\mathbf{h}, \mathbf{r}) &= \sum_{k=1}^{K_j} w_j(k) \, f(\boldsymbol{g}_{j,k}) \, (\mathcal{R}[G_j(\cos \frac{\omega(\boldsymbol{g}', \circ)}{2})])(\mathbf{h}, \mathbf{r}) \\ &= \sum_{k=1}^{K_j} w_j(k) \, f(\boldsymbol{g}_{j,k}) \, (\mathcal{R}G_j)(\boldsymbol{g}_{j,k}\mathbf{h} \cdot \mathbf{r}) \\ &= \sum_{k=1}^{K_j} w_j(k) \, f(\boldsymbol{g}_{j,k}) \, \widetilde{G}_j(\boldsymbol{g}_{j,k}\mathbf{h} \cdot \mathbf{r}) \end{aligned} \quad (25)$$

as Eq. (7) implies

$$\left(\mathcal{R}[C_\ell^{(1)}(\boldsymbol{g}_0^{-1} \circ)]\right)(\mathbf{h}, \mathbf{r}) = P_\ell(\boldsymbol{g}_0 \mathbf{h} \cdot \mathbf{r}). \quad (26)$$

Comparing Eq. (25) with Eq. (14) we may be led to identify first $\boldsymbol{g}_{j,k}\mathbf{h}$ with $\mathbf{r}'_{j,k}$ and further $w_j(k) \, f(\boldsymbol{g}_{j,k})$ with $w'_j(k) \, (\mathcal{R}f)(\mathbf{h}, \mathbf{r}'_{j,k})$. Analogous results are valid for $(\mathcal{R}[S_{W_j}^I f(\circ)])(\mathbf{h}, \mathbf{r})$ with respect to $S_{W_j}^I (\mathcal{R}f)(\mathbf{h}, \mathbf{r})$ .

Thus, roughly speaking, averaging an orientation probability density function along circles of $SO(3)$ parametrized by $\mathbf{h}, \mathbf{r} \in S^2$ interchanges with its wavelet approximation: The spherical Radon transform of the wavelet representation of an orientation probability density function

is the wavelet representation of its Radon transform, the pole probability density functions. In practical applications, initially approximating experimental pole figure intensities by spherical wavelets according to Eq. (14) eventually results in the corresponding wavelet approximation Eq. (24) of the even part of an orientation probability density function explaining the data.

## Applications

High resolution texture analysis is required in quality control of high–tech materials where the ultimate goal is a perfect "single crystal" preferred orientation, as in high–temperature semi–conductors where the mean deviation from the "single crystal" peak orientation must not be larger than 1 degree. Similar problems arise in the analysis of "bamboo–structures" of single crystal wide copper wires on silicon wavers, or in thin epitaxial superconducting films, the electrical and magnetic properties of which are critical for their performance as electronic devices and need to be optimized.

Methods of high resolution texture analysis may also be required to resolve the "orientation distribution of single crystals" observed in recent synchrotron radiation experiments (Wenk [10]).

Another example, maybe less spectacular but as demanding is the resolution of the mixture of a (100) and a (110) fibre–distribution with a ratio of peak intensities of 2 to 1 in hexagonal crystal symmetry, where high resolution texture analysis is required (Chateigner [2]).

## Conclusions

The main idea of wavelet analysis is to obtain a multiscale representation of the data or functions which allows localization in space and frequency. In particular, the spherical wavelet representation of pole probability density functions corresponds to a hyperspherical wavelet representation of orientation probability density functions and vice versa. Thus, multiscale representation is transferred from one to the other and applies simultaneously.

The representation of diffraction pole figures and orientation probability density functions by spherical wavelets

- is well suited to render pole and orientation probability density functions,
- provides a multiscale representation which allows for localization in frequency and space domain, i.e. adjusted to a locally refined grid according to large variations in the recorded pole figure intensities,
- provides means for a self–adaptive control of a texture goniometer adjusting the scan to a grid refinement in areas of large intensity variations,
- applies to the solution of the inverse texture problem due to the correspondence of the multiscale representation of pole and orientation probability density functions by virtue of (generalized) spherical wavelets.

Thus, spherical wavelets provide an appropriate means for high resolution texture analysis.

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