TECHNISCHE UNIVERSITÄT BERGAKADEMIE FREIBERG

Die Ressourcenuniversität. Seit 1765.

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The crystallographic Radon transform and diffusive wavelets

New Trends and Directions in Harmonic Analysis, Fractional Operator Theory and Image Analysis, Inzell, Germany, September 17 -21, 2012



Motivation

Texture analysis is the analysis of the statistical distribution of orientations of crystals within a specimen of a polycrystalline material, which could be metals or rocks. The crystallographic orientation g of an individual crystal is the active rotation $g \in SO(3)$ that maps a co-ordinate system fixed to the specimen onto another co-ordinate system fixed to the crystal.



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Orientation density function

The orientation distribution by volume ΔV_g requires a measure of the volume portion $\frac{\Delta V_g}{V}$ of total volume V carrying crystal gains with orientations within a volume element $\Delta G \subset G$ of the subgroup G of all feasible $G \in SO(3)$.

$$\frac{\Delta V_g}{V} \to f(g) \, dg$$



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Goniometer



classical goniometer



4-circle-goniometer

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Pole density function

- odf cannot be directly measured,
- only pole density functions (pdf) P(h,r) can be sampled,
- Iet be

$$(\mathscr{R}f)(h,r) = 4\pi \int_{\{g \in SO(3):h=gr\}} f(g) \, dg$$

= $4\pi \int_{SO(3)} f(g) \delta_r(g^{-1h}) \, dg = (f * \delta_r),$

it represents that a fixed crystal direction \boldsymbol{h} statistically coincides with the specimen direction \boldsymbol{r}

Due to Friedel's law which says that the X-ray cannot distinguish between the top and the bottom of the lattice planes, we are only able to measure a mean value which correspondence to a negligence of the orientation on SO(3), i.e. the pdf

$$P(h,r) = \frac{1}{2} \left((\mathscr{R}f)(h,r) + (\mathscr{R}f)(-h,r) \right).$$

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PDF



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Crystallographic Radon transform

Problem (Analytic reconstruction problem)

Reconstruct the ODF f(g), $g \in SO(3)$, from all pole figures P(h,r), $h,r \in S^2$. Because f(g) is an ODF we have two additional conditions:

1. $f(g) \ge 0$, i.e. f is non-negative,

2.
$$\int_{SO(3)} f(g) dg = 1.$$

Problem (Totally geodesic Radon transform on SO(3))

Reconstruct $f(g), g \in SO(3)$, from all $\mathscr{R}(h,r), h, r \in S^2$.

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Crystallographic Radon transform

Radon-Transformation

$$(\mathscr{R}f)(h, r) := \int_{\{g \in SO(3): gh = r\}} f(g) \, dg$$

= $\int_{SO(3)} f(g) \, \delta_h(g^{-1}r) \, dg = f * \delta_{h, r}$
= $\int_{SO(2)} f(rlh^{-1}) dl,$

because a great circle $C_{h,r}$ can be described that way.

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Let $\hat{\mathscr{G}}$ denote the set of all equivalence classes of irreducible representations. Then this set parametrerizes an orthogonal decomposition of $L^2(\mathscr{G})$.

Theorem (Peter-Weyl)

Let \mathscr{G} be a compact Lie group. Then the following statements are true.

• Denote $H_{\pi} = \{g \mapsto \operatorname{trace}(\pi(g)M) : M \in \mathbb{C}^{d_{\pi} \times d_{\pi}}\}$. Then the Hilbert space $L^{2}(\mathscr{G})$ decomposes into the orthogonal direct sum

$$L^2(\mathscr{G}) = \bigoplus_{\pi \in \hat{\mathscr{G}}} H_{\pi}$$

• For each irreducible representation $\pi \in \hat{\mathscr{G}}$ the orthogonal projection $L^2(\mathscr{G}) \to H_{\pi}$ is given by

$$f \mapsto d_{\pi} \int_{\mathscr{G}} f(h) \chi_{\pi}(h^{-1}g) \, dh = d_{\pi} f * \chi_{\pi},$$

in terms of the character $\chi_{\pi}(g) = \operatorname{trace}(\pi(g))$ of the representation and dh is the normalized Haar measure.

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• the matrix M in the equation $f * \chi_{\pi} = \operatorname{trace}(\pi(g)M)$ are the Fourier coefficient $\hat{f}(\pi)$ of f at the irreducible representation π .

•
$$\widehat{f}(\pi) = \int_{\mathscr{G}} f(g) \pi^*(g) \, dg$$

• inversion formula (the Fourier expansion)

$$f(g) = \sum_{\pi \in \hat{\mathscr{G}}} d_{\pi} \operatorname{trace}(\pi(g)\hat{f}(\pi))$$

If we denote by $||M||^2_{HS}=\mathrm{trace}(M^*M)$ the Frobenius or Hilbert-Schmidt norm of a matrix M, then the following Parseval identity is true.

Lemma (Parseval identity)

Let $f \in L^2(\mathscr{G})$. Then the matrix-valued Fourier coefficients $\hat{f} \in \mathbb{C}^{d_\pi \times d_\pi}$ satisfy

$$||f||^2 = \sum_{\pi \in \widehat{\mathscr{G}}} d_\pi \, ||\widehat{f}(\pi)||^2_{HS}.$$

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Definition

Let \mathscr{H} be a subgroup of the compact Lie group \mathscr{G} . The Radon transform \mathscr{R} of an integrable function f on \mathscr{G} is defined by

$$\mathscr{R}f(x,y) = \int_{\mathscr{H}} f(xhy^{-1}) \, dh, \quad x, y \in \mathscr{G}, \tag{1}$$

where dh denotes the normalized Haar measure on \mathcal{H} .

Lemma (B./Ebert/Pesenson - 2012)

The Radon transform (1) is invariant under right shifts of x and y, hence the range is a subset of $\mathscr{G}/\mathscr{H} \times \mathscr{G}/\mathscr{H}$.

Theorem (B./Ebert/Pesenson - 2012)

Let \mathscr{H} be a subgroup of \mathscr{G} which determines the Radon transform on \mathscr{G} and let $\hat{\mathscr{G}}_1 \subset \hat{G}$ be the set of irreducible representations with respect to \mathscr{H} . Then for $f \in C^{\infty}(\mathscr{G})$ we have $||\mathscr{R}||^2_{L^2(\mathscr{G}/\mathscr{H} \times \mathscr{G}/\mathscr{H})} = \sum \operatorname{rank}(\pi_{\mathscr{H}})||\hat{f}||^2_{HS}.$

 $\pi \in \hat{\mathscr{G}}$

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Hilbert space structure

We want to find a Hilbert space structure such that the Radon transform is an isometry, which means that

$$\begin{split} ||f||_{L^{2}(\mathscr{G})}^{2} &= \sum_{\pi \in \hat{\mathscr{G}}} d_{\pi} ||\hat{f}(\pi)||_{HS}^{2} \\ \sum_{\pi \in \hat{\mathscr{G}}} d_{\pi} ||\hat{f}(\pi)||_{L^{2}(\mathscr{G}/\mathscr{H} \times \mathscr{G}/\mathscr{H})}^{2} &= |||\mathscr{R}f|||_{L^{2}(\mathscr{G}/\mathscr{H} \times \mathscr{G}/\mathscr{H})}^{2} \end{split}$$

Lemma (Taylor, 1986)

If \mathcal{M} is a compact rank one symmetric space, then \mathscr{G} acts irreducibly on each eigenspace V_{λ} of Δ on \mathcal{M} .

Examples of such compact rank one symmetric spaces are

$$\mathscr{G} = SO(n+1), \quad \mathcal{M} = S^n,$$

 $\mathscr{G} = SU(n+1), \quad \mathcal{M} = \mathbb{C}P^n$ (complex projective plane

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Definition

A representation l(g) is called a representation of class-1 relative to \mathscr{H} if in its space there are nonzero vectors invariant relative to \mathscr{H} and the restriction of l(g) to \mathscr{H} is unitary.

Lemma

If $\mathcal{M} = \mathcal{G}/\mathcal{H}$ is a rank one symmetric space, with \mathcal{H} connected, than $L^2(\mathcal{M})$ contains each class-1 representation, exactly once, as an eigenspace of Δ .

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Spherical harmonics and Wigner polynomials

- orthonormal system of spherical harmonics $\mathcal{Y}_k^i \in C^{\infty}(S^n), \ k \in \mathbb{N}_0, \ i = 1, \dots, d_k(n)$ normalized with respect to the Lebesgue measure on S^n .
- Then the Wigner polynomials on SO(n+1) $\mathcal{T}_k^{ij}(g), \ g \in SO(n+1)$ are given by

$$\mathcal{T}_k^{ij}(g) = \int_{S^n} \mathcal{Y}_k^i(g^{-1}x) \overline{\mathcal{Y}_k^j(x)} \, dx$$

$$\mathcal{Y}_k^i(g^{-1}x) = \sum_{j=1}^{d_k(n)} \mathcal{T}_k^{ij}(g) \mathcal{Y}_k^j(x).$$

- Wigner polynomials build an orthonormal system in $L^2(SO(n+1))$.
- Unfortunately, Wigner polynomials do not give all irreducible unitary representations of SO(n+1) if $n \ge 2$.

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Projections

We look for all representations of SO(n+1) which do not have vanishing coefficients under the projection with respect to SO(n), these are the class-1 representations of SO(n+1):

 x_0 is the base point of $SO(n+1)/SO(n)\sim S^n,$ $\mathcal{C}_k^{(n-1)/2}$ are the Gegenbauer polynomials.

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Radon transform from $span(\mathcal{T}_k)$ into $S^n \times S^n$

Let be

$$f(g) = \sum_{k=0}^{\infty} \sum_{i,j=1}^{d_k(n)} \hat{f}(k)_{ij} \mathcal{T}_k^{ij}.$$

then

$$\begin{aligned} (\mathscr{R}f)(h,r) &= \sum_{k=0}^{\infty} d_k(n) \operatorname{trace} \left(\widehat{f}(k) \mathcal{T}_k(h) \pi_{SO(n)} \mathcal{T}_k^*(r) \right) \\ &= \sum_{k=0}^{\infty} d_k(n) \sum_{i,j=1}^{d_k(n)} \widehat{f}(k)_{ij} \mathcal{T}_k^{i1}(h) \overline{\mathcal{T}_k^{1j}(r)} \\ &= \sum_{k=0}^{\infty} \frac{|S^n|}{d_k(n)} d_k(n) \sum_{i,j=1}^{d_k(n)} \widehat{f}(k)_{ij} \mathcal{Y}_k^i(h) \overline{\mathcal{Y}_k^j(r)} \\ &= |S^n| \sum_{k=0}^{\infty} \sum_{i,j=1}^{d_k(n)} \widehat{f}(k)_{ij} \mathcal{Y}_k^i(h) \overline{\mathcal{Y}_k^j(r)} \end{aligned}$$

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Mapping properties

- $\Delta_h(\mathscr{R}f) = \Delta_r(\mathscr{R}f)$
- For g = Rf the Fourier coefficients fulfill $\hat{g}(k)_{ij} = |S^n|\hat{f}(k)_{ij}$

The crystallographic Radon transform maps Wigner poynomials, i.e. span (\mathcal{T}_k) , onto span $(\mathcal{Y}_k^i \overline{\mathcal{Y}_k^j})$.

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The case SO(3)

Lemma (Taylor, 1986)

The decomposition

$$L^2(S^2) = \bigoplus_k V_k$$

contains each irreducible unitary representation of SO(3), exactly once. Choosing $\mathscr{G} = SO(3)$, $\mathscr{H} = SO(2)$ and thus $\mathscr{G}/\mathscr{H} = SO(3)/SO(2) = S^2$, all irreducible representations are equivalent to an irreducible component of the left regular representation

$$T(g): f(x) \mapsto f(g^{-1} \cdot x),$$

where \cdot denotes the canonical action of SO(3) on S^2 . The T invariant subspaces of $L^2(S^2)$ are $\mathcal{H}_k = \{\mathcal{Y}_k^i, i = 1, \dots, 2k+1\}$, which are spanned by all spherical harmonics of degree k. The dimension of the representations space is $d_k = 2k+1$ and $-\lambda_k^2 = -k(k+1)$ we get

$$d_k = \sqrt{1+4\lambda_k^2} \text{ and } \sqrt{d_k} = \sqrt[4]{(2(\lambda_k^2+\lambda_k^2)+1)}.$$

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Hilbert space structure

Parseval's identity

$$||f||^2_{L^2(SO(3))} = \sum_{k=1}^{\infty} (2k+1) ||\hat{f}(k)||^2_{HS}.$$

Because of Δ on S^2 is equal to -k(k+1) on the representation space = eigenspace \mathcal{H}_k of the Laplacian we obtain

$$=\sum_{k=1}^{\infty} (2k+1)||4\pi \hat{f}(k)||_{L^{2}(S^{2}\times S^{2})}^{2} = ||4\pi(-2(\Delta_{1}+\Delta_{2})+1)^{1/4}\mathscr{R}f||_{L^{2}(S^{2}\times S^{2})}^{2},$$

where $\Delta_1 + \Delta_2$ is a Laplace operator on $S^2 \times S^2$. Thus we define the following norm for $u \in C^{\infty}(S^2 \times S^2)$

$$|||u|||^{2} = (4\pi)^{2} ((-2\Delta_{S^{2} \times S^{2}} + 1)^{1/2} u, u)_{L^{2}(S^{2} \times S^{2})},$$

where $\Delta_{S^2 \times S^2} = \Delta_1 + \Delta_2$.

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Sobolev spaces

Definition

The Sobolev space $H_t(S^2 \times S^2)$, $t \in \mathbb{R}$, is defined as the domain of the operator $(1 - 2\Delta_{S^2 \times S^2})^{\frac{t}{2}}$ with graph norm

$$||f||_t = ||(1 - 2\Delta_{S^2 \times S^2})^{\frac{t}{2}} f||_{L^2(S^2 \times S^2)}, \ f \in L^2(S^2 \times S^2).$$

The Sobolev space $H_t^{\Delta}(S^2 \times S^2)$, $t \in \mathbb{R}$, is defined as the subspace of all functions $f \in H_t(S^2 \times S^2)$ such $\Delta_1 f = \Delta_2 f$.

Definition

The Sobolev space $H_t(SO(3)), t \in \mathbb{R}$, is defined as the domain of the operator $(1 - 4\Delta_{SO(3)})^{\frac{t}{2}}$ with graph norm

$$|||f|||_t = ||(1 - 4\Delta_{SO(3)})^{\frac{t}{2}}f||_{L^2(SO(3))}, \ f \in L^2(SO(3)).$$

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Theorem (Range description, B./Ebert/Pesenson, 2012) For any $t \ge 0$ the Radon transform on SO(3) is an invertible mapping $\mathscr{R}: H_t(SO(3)) \to H^{\Delta}_{t+\frac{1}{2}}(S^2 \times S^2).$ (2)

Proof: It is sufficient to consider case t = 0.

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Grouptheoretical approach

Wavelets are coherent states.

Consider the affine group of translations and dilations acting on the real line. Let \mathcal{M} be a Riemannian manifold. A wavelet transform in $L^2(\mathcal{M})$ is defined in terms of an unitary representation U of Lie group \mathcal{G}

$$U: \mathcal{G} \to \mathcal{L}(L^2(\mathcal{M})).$$

A non-zero vector $\Psi\in L^2(\mathcal{M})$ is an admissible wavelet if

$$\int_{\mathcal{G}} |\langle f, \, U(g)\Psi\rangle_{L^2(\mathcal{M})}|^2 \, dg < \infty$$

for all $f \in L^2(\mathcal{M})$. The associated wavelet transform is

$$\mathcal{W}f(g) = \langle f, U(g)\Psi \rangle_{L^2(\mathcal{M})}$$

bounded and invertible on its range.

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Grouptheretical approach – drawbacks

- Because L²(M) is infinite dimensional, no compact group admits an irreducible unitary representation of this form.
- However, compact groups seem natural at least in the situation where \mathcal{M} itself is a homogeneous space of a compact group. For example $\mathbb{S}^2 = SO(3)/SO(2)$.
- Spheres: Irreducible representation of that form are not square integrable and hence one cannot find an admissible wavelet.



Alternative approaches

Classical wavelet theory (in \mathbb{R}^n) is based on the group generated by translations and dilations.

Translations on a sphere (seen as a homogeneous space of rotations) are rotations.

What are dilations?

Key idea: generate dilations from a diffusive semigroup, e.g., from time-evolution of solutions to a heat equation on a homogeneous space.

W. Freeden, T. Gervens, and M. Schreiner, *Constructive Approximation on the Sphere with Applications to Geomathematics*, Oxford Univ. Press, Oxford, 1999.

Discrete wavelet transforms in such a setting:

R. Coifman, M. Maggioni, *Diffusion wavelets*, Appl. Comp. Harm. Anal. 21(1):53-94, 2006.

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Diffusive wavelets - General philosophy

Let $p_t \in L^1(G)$ be an approximate convolution identity, i.e. $\varphi * p_t \to \varphi$ as $t \to 0$ for all $\varphi \in L^2(G)$. Assign families $\psi_{\rho}, \Psi_{\rho} \in L^1(G)$ to p_t such that

$$p_t = \int_t^\infty \check{\psi}_\rho * \Psi_\rho \,\alpha(\rho) \,d\rho.$$

We assign to φ a two-parameter function $W\varphi,$ the Wavelet transform $\varphi(g)\mapsto W\varphi(\rho,\,g),$

$$W\varphi(\rho, g) = \varphi * \check{\psi}_{\rho} = \int_{G} \varphi(h) \check{\psi}_{\rho}(h^{-1}g) \, d\mu_{G}(h) = \langle \varphi, T_{g}\psi_{\rho} \rangle,$$

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Diffusive wavelets - General philosophy

and the inversion formula

$$\varphi = \int_{\to 0}^{\infty} W\varphi(\rho, \cdot) * \Psi_{\rho} \, \alpha(\rho) \, d\rho = \varphi * \int_{\to 0}^{\infty} \check{\psi}_{\rho} * \Psi_{\rho} \, \alpha(\rho) \, d\rho.$$

Of interest are in particular those for which the operator $*\partial_t p_t$ is positive. Then the corresponding Fourier coefficients are positive matrices and the choice $\psi_{\rho} = \Psi_{\rho}$ seems reasonable.

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Diffusive approximate identity

Definition

Let $\hat{G}_+ \subset \hat{G}$ be cofinite. A family $t \to p_t$ from $C^1(\mathbb{R}_+; L^1(G))$ will be called diffusive approximate identity with respect to \hat{G}_+ if it satisfies

- $||\hat{p}_t(\pi)|| \leq C$ uniform in $\pi \in \hat{G}_+$ and $t \in \mathbb{R}_+$;
- $\lim_{t\to 0} \hat{p}_t(\pi) = I$ for all $\pi \in \hat{G}_+$;
- $\lim_{t\to\infty} \hat{p}_t(\pi) = 0$ for all $\pi \in \hat{G}_+$;
- $-\partial_t \hat{p}_t(\pi)$ is a positive matrix for all $t \in \mathbb{R}_+$.

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Definition

Let p_t be a diffusive approximate identity and $\alpha(\rho) > 0$ a given weight function.

A family $\psi_{\rho} \in L^2_0(G) = \bigoplus_{\pi \in \hat{G}_+} H_{\pi}$ is called diffusive wavelet family, if it satisfies the admissibility condition

$$p_t|_{\hat{G}_+} = \int_t^\infty \check{\psi}_\rho * \psi_\rho \,\alpha(\rho) \,d\rho.$$

This equation can be solved explicitely. Applying Fourier transform to both sides and by differentiating both sides yields

$$-\partial_t \hat{p}_t(\pi) = \hat{\psi}_\rho(\pi) \hat{\psi}_\rho^*(\pi) \alpha(\rho).$$

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Heat wavelet family

If p_t is the heat kernel we get

$$\hat{\psi}_{\rho}(\pi) = \frac{1}{\sqrt{\alpha(\rho)}} \lambda_{\pi} e^{-\rho \lambda_{\pi}^2/2} \eta_{\pi}(\rho)$$

for any (fixed) choice of a family $\eta_{\pi}(\rho) \in U(d_{\pi})$. This implies

$$\psi_{\rho} = \frac{1}{\sqrt{\alpha(\rho)}} \sum_{\pi \in \hat{G}} d_{\pi} \lambda_{\pi} e^{-\rho \lambda_{\pi}^2/2} \operatorname{trace}\left(\pi(g)\eta_{\pi}(\rho)\right).$$

The weight function $\alpha(\rho)$ can be used to normalize the family ψ_{ρ} .

$$\alpha(\rho) = -\Delta_G p_\rho(1),$$

where $p_{\rho}(1)$ is just the heat trace on G.

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Diffusive wavelets on homogeneous spaces G/H

We have two options to construct wavelets on homogeneous spaces:

The naive way: We apply the wavelet transform to the lifted function $\tilde{\varphi}(g) = \varphi(g \cdot x_0)$ with base-point $x_0 \in X = G/H$ for some $\varphi \in L^2(X)$. This defines a function on $\mathbb{R}_+ \times G$ via

$$W\tilde{\varphi}(\rho,g) = \int_{G} \tilde{\varphi}(h)\check{\psi}_{\rho}(h^{-1}g) \, d\mu_{G}(h) = \int_{G} \varphi(h \cdot x_{0})\check{\psi}_{\rho}(h^{-1}g) \, d\mu_{G}(h)$$

But we would prever to have a transform living on $\mathbb{R}_+\times X$ instead of $\mathbb{R}_+\times G.$

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Diffusive wavelets on homogeneous spaces X = G/H

Let p_t be a diffusive approximate identity and $\alpha(\rho) > 0$ be a given weight function. A family $\psi_{\rho} \in L^2(X)$ is called a diffusive wavelet family if the admissibility condition

$$p_t^X(x)\Big|_{\hat{G}_+} = \int_t^\infty \psi_\rho \bullet \psi_\rho(x) \,\alpha(\rho) \,d\rho$$

is satiesfied. We associate to this family the wavelet transform

$$W_X \varphi(\rho, g) = \varphi \bullet \psi_\rho(g) = \int_X \varphi(x) \overline{\psi(g^{-1} \cdot x)} \, dx$$

with inverse given as

$$\tilde{\varphi} = \int_{\to 0}^{\infty} W_X \varphi(\rho, \cdot) * \tilde{\psi}_{\rho} \, \alpha(\rho) \, d\rho \quad \text{for all} \quad \varphi \in L^2_0(X).$$

$$\begin{split} \varphi \ast \psi(x) &= \int_{G} \varphi(g \cdot x_{0}) \psi(g^{-1} \cdot x) \, d\mu_{g} \in L^{1}(X), & \widetilde{\varphi} \ast \widetilde{\psi} = \widetilde{\varphi} \ast \widetilde{\psi} \\ \varphi \bullet \psi(x) &= \int_{X} \overline{\varphi(g \cdot x_{0})} \psi(g \cdot x) \, d\mu_{g} = \langle \varphi, \, T_{g} \psi \rangle \in L^{1}(G), & \varphi \bullet \psi = \check{\varphi} \ast \check{\psi}, \\ \varphi \bullet \psi(g) &= \int_{X} \varphi(x) \overline{\psi(g^{-1} \cdot x)} \, dx \in L^{1}(X), & \varphi \bullet \psi = \tilde{\varphi} \ast \check{\psi}. \end{split}$$

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Theorem (Wavelets from wavelets)

Let $\{\Psi_{\rho}, \rho > 0\}$ be a family of class type wavelets $(\eta_{\rho}(\pi) = I)$ on SO(3), then the family of function $\{R\Psi_{\rho}(x,.), \rho > 0, x \in S^2 fixed\}$ defines a family of zonal wavelets on S^2 .

If we make a non-trivial choice $\eta_{\rho}(\pi) \neq 0$, we obtain non-zonal wavelets.

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Thank you for your attention!

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