A one-dimensional Radon transform on $\text{SO}(3)$ and its application to texture goniometry

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1 Introduction

1.1 Motivation from texture goniometry

Texture analysis with X-ray diffraction data is the analysis of the orientation distribution by volume and asks for a measure of the volume portion $\Delta V/V$ of a polycrystalline specimen of total volume $V$ carrying crystal grains with orientations within a range (volume element) $\Delta G \subset G$ of the subgroup $G$ of all feasible orientations $G \subset \text{SO}(3)$.

The orientation $g$ of an individual crystal in a polycrystalline specimen is the active rotation $g \in \text{SO}(3) : K_S \mapsto K_C$ that maps a right–handed orthonormal coordinate system $K_S$ fixed to the specimen onto another right–handed orthonormal coordinate system $K_C$ fixed to the crystal,

$$g K_S = K_C, \ g \in \text{SO}(3).$$

If a unique direction is represented by unit vector $h$ with respect to the crystal frame $K_C$, and by unit vector $r$ with respect to the specimen frame $K_S$, then the coordinates of the unique direction transform according to

$$r_{K_S} = g h_{K_C}.$$  \hspace{1cm} (2)

The commonly applied convention in texture analysis (H.J. Bunge, [1]; [2]) refers to the notion of passive rotation and Eq. 2 is written in the form

$$h = gr$$  \hspace{1cm} (3)

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where obviously $g = g^{-1}$. Since we aim at a unified view of inversion formulae developed in such apparently diverse fields as texture analysis, integral geometry, and spherical tomography, we use here the notation Eq. 3 familiar in applied sciences. Thus, it is our hope to accomplish clarification without confusion by yet another convention.

Assuming that the measure possesses a probability density function $f : G \mapsto \mathbb{R}_+$, then

\[ \text{prob}(g \in \Delta G) = \int_{\Delta G} f(g) \, d\omega_g \]

and $f$ is referred to as the orientation density function by volume and $d\omega_g = \sin \beta \, d\alpha \, d\beta \, d\gamma$ is the usual Riemannian measure of $\mathbb{S}^3$ which differs from the invariant Haar measure $dg$ of $\text{SO}(3)$ by a constant factor, we have $d\omega_g = 8\pi^2 \, dg$.

In X-ray diffraction experiments the orientation density function $f$ cannot be directly measured but with a texture goniometer only pole density function $P(h, r)$ can be sampled, which represents the probability that a (fixed) crystal direction $h$ or its antipodal $-h$ statistically coincide with the specimen direction $r$. With respect to the experiment the feasible crystal directions are the normals of the crystallographic lattice planes. A pole density function is the tomographic projection of an orientation density function which is basically provided by

\[ P f(h, r) = \frac{1}{2} (R(h, r) + R(-h, r)) \]

with

\[ R f(h, r) = \frac{1}{2\pi} \int_{\{g \in \text{SO}(3) \mid h = g \cdot r\}} f(g) \, d\omega_g \]

\[ = 4\pi \int_{\text{SO}(3)} f(g) \delta_r(g^{-1} \cdot h) \, dg = (f * \delta_r)(h). \]

## 2 Main results

We start with the one-dimensional Radon transform on $\text{SO}(3)$ and its inversion. Using a group-theoretical approach we will obtain an inversion formula which will be the basis for other inversion formulae. An important tool will be the series expansions in surface harmonics on $\mathbb{S}^2 \times \mathbb{S}^2$ as well as in rotational harmonics on $\text{SO}(3)$.

Let $f \in L^2(\text{SO}(3))$. We define the Fourier series on $\text{SO}(3)$ by

\[ f(g) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} (2l+1) \hat{f}_{lmn}^l (D_{m,n}^l)(g) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} (2l+1) \hat{f}_{lmn}^l D_{m,n}^l(g^{-1}), \]

where

\[ \hat{f}_{lmn}^l = \int_{\text{SO}(3)} f(g) \, D_{m,n}^l(g) \, dg, \quad -l \leq m, n \leq l, \quad l = 0, 1, \ldots \]

and $dg$ is the Haar measure on $\text{SO}(3)$. 
Therefore we get
\[ \mathcal{F}_{SO(3)} f = 4\pi \mathcal{F}_{S^2 \times S^2} (\mathcal{R} f), \]
i.e. the Fourier coefficients of \( f \) in \( L^2(\text{SO}(3)) \) are equal to \( 4\pi \)-times the Fourier coefficients of \( \mathcal{R} f \) in \( L^2(S^2 \times S^2) \). Furthermore, we have several inversion formulae
\[ f(g) = 4\pi \check{\mathcal{R}} (-2\Delta_{S^2 \times S^2} + 1)^{1/2} \mathcal{R} f \]
(4)
\[ = 4\pi (-4\Delta_{SO(3)} + 1)^{1/2} \check{\mathcal{R}} \mathcal{R} f \]
(5)
\[ = \frac{1}{4\pi} \left\{ \int_{S^2} \mathcal{R}(h, -g h) \, dS^2_h + 2 \int_0^{\pi} \cos \theta \frac{d}{d\cos \theta} \int_{S^2} (W f)(h, g h, \cos \theta) \, dS^2_h \, d\theta \right\}, \]
(6)
where \( \check{\mathcal{R}} \) denotes the dual Radon transform in \( L^2 \).

Formula (4) is the starting point of all other inversion formulae which are derived by series expansion into spherical harmonics and rotational spherical harmonics. The second formula (5) is the analog of the so-called backprojection formula in the Euclidean case and could be used to detect edges and wedges. The third formula is of special interest because it occurs in crystallographic literature see for example [1], [2], [5].

Further we demonstrate its equivalence to the inversion formula of the spherical Radon transform on \( S^3 \) given by S. Helgason ([3], [4]).

The X-ray transform in texture goniometry differs from the Radon transform on \( \text{SO}(3) \) in the following way. Due to Friedel’s law which states 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 \( \text{SO}(3) \). Therefore the X-ray transform in texture goniometry is not an isomorphism.

References

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